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BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK,
EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN,
IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV,
MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU,
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ance Notes on Codes and Abbreviations" appearing at the begin-
ning of each regular issue of the PCT Gazette.

(54) Title: TERPENE SYNTHASES

(57) Abstract: Novel synthases and the corresponding nucleic acids encoding such synthases are disclosed herein. Such synthases possess an active site pocket that includes key amino acid residues that are modified to generate desired terpenoid reaction intermediates and products. Synthase modifications are designed based on, e.g., the three-dimensional coordinates of tobacco 5-cpi-aristolochene synthase, with or without a substrate bound in the active site.

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INTERNATIONAL SEARCH REPORT

International Application No
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A. CLASSIFICATION OF SUBJECT MATTER

IPC 7 C12N9/10 C07K14/415 C12N15/54 C12N15/29 C12N9/88

According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)

IPC 7 C12N C07K

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practical, search terms used)

C. DOCUMENTS CONSIDERED TO BE RELEVANT

| Category * | Citation of document, with indication, where appropriate, of the relevant passages | Relevant to claim No. |
|------------|--|-----------------------|
| X | STARKS, C.M. ET AL: "Structural basis for cyclic terpene biosynthesis by tobacco 5-epi-aristolochene synthase" SCIENCE, vol. 277, 19 September 1997 (1997-09-19), pages 1815-1820, XP000867114 LANCASTER US the whole document | 1-94 |
| X | WO 97 38703 A (UNIVERSITY OF KENTUCKY) 23 October 1997 (1997-10-23) the whole document --- -/-- | 95-101, 144,153 |

☒ Further documents are listed in the continuation of box C.

☒ Patent family members are listed in annex.

* Special categories of cited documents :

- *A* document defining the general state of the art which is not considered to be of particular relevance
- *E* earlier document but published on or after the international filing date
- *L* document which may throw doubts on priority claim(s) or which is cited to establish the publication date of another citation or other special reason (as specified)
- *O* document referring to an oral disclosure, use, exhibition or other means
- *P* document published prior to the international filing date but later than the priority date claimed

T later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention

X document of particular relevance: the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone

Y document of particular relevance: the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art.

G document member of the same patent family

Date of the actual completion of the international search

9 February 2000

Date of mailing of the international search report

23. MAI 2000

Name and mailing address of the ISA

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C.(Continuation) DOCUMENTS CONSIDERED TO BE RELEVANT

| Category * | Citation of document, with indication, where appropriate, of the relevant passages | Relevant to claim No. |
|------------|--|-----------------------|
| A | <p>LESBURG C.A. ET AL.: "Crystal structure of pentalene synthase: mechanistic insights on terpenoid cyclization reactions in biology" SCIENCE., vol. 277, no. 5333, 19 September 1997 (1997-09-19), pages 1820-1824, XP000867083 LANCASTER US the whole document</p> | 1 |
| A | <p>MAU C.J.D. ET AL.: "Cloning of casbene synthase cDNA: evidence for conserved structural features among terpenoid cyclases in plants" PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF USA., vol. 91, August 1994 (1994-08), pages 8497-8501, XP002130098 WASHINGTON US ISSN: 0027-8424 the whole document</p> | 1 |
| A | <p>PETER FACCHINI ET AL: "Gene family for an elicitor-induced sesquiterpene cyclase in tobacco" PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF USA,US,NATIONAL ACADEMY OF SCIENCE. WASHINGTON, vol. 89, no. 89, page 11088-11092-11092 XP002102270 ISSN: 0027-8424 the whole document</p> | 1 |
| A | <p>WO 96 36697 A (UNIVERSITY OF KENTUCKY) 21 November 1996 (1996-11-21) page 19, line 1 -page 44, line 14</p> | 1 |
| P,X | <p>LESBURG C.A. ET AL.: "Managing and manipulating carbocations in biology: Terpenoid cylase structure and mechanism" CURRENT OPINION IN STRUCTURAL BIOLOGY., vol. 8, no. 6, December 1998 (1998-12), pages 695-703, XP000874866 LONDON GB ISSN: 0959-440X the whole document</p> | 1 |

INTERNATIONAL SEARCH REPORT

International application No.
PCT/US 99/21419

Box I Observations where certain claims were found unsearchable (Continuation of item 1 of first sheet)

This International Search Report has not been established in respect of certain claims under Article 17(2)(a) for the following reasons:

1. ☐ Claims Nos.:
because they relate to subject matter not required to be searched by this Authority, namely:
2. ☒ Claims Nos.:
because they relate to parts of the International Application that do not comply with the prescribed requirements to such an extent that no meaningful International Search can be carried out, specifically:
see FURTHER INFORMATION sheet PCT/ISA/210
3. ☐ Claims Nos.:
because they are dependent claims and are not drafted in accordance with the second and third sentences of Rule 6.4(a).

Box II Observations where unity of invention is lacking (Continuation of item 2 of first sheet)

This International Searching Authority found multiple inventions in this international application, as follows:

1. ☐ As all required additional search fees were timely paid by the applicant, this International Search Report covers all searchable claims.
2. ☐ As all searchable claims could be searched without effort justifying an additional fee, this Authority did not invite payment of any additional fee.
3. ☐ As only some of the required additional search fees were timely paid by the applicant, this International Search Report covers only those claims for which fees were paid, specifically claims Nos.:
4. ☒ No required additional search fees were timely paid by the applicant. Consequently, this International Search Report is restricted to the invention first mentioned in the claims; it is covered by claims Nos.:

1-101, 119-128, 129-132 PARTLY, 133-151, 153-162

Remark on Protest

- ☐ The additional search fees were accompanied by the applicant's protest.
- ☐ No protest accompanied the payment of additional search fees.

FURTHER INFORMATION CONTINUED FROM PCT/ISA/ 210

Continuation of Box I.2

Present claims 1-101, 119-151, 153-162 relate to an extremely large number of possible compounds i.e. terpene synthases. In fact, the claims contain so many options, variables, possible permutations and provisos that a lack of clarity (and/or conciseness) within the meaning of Article 6 PCT arises to such an extent as to render a meaningful search of the claims impossible. Consequently, the search has been carried out for those parts of the application which do appear to be clear (and/or concise), namely those terpene synthases recited in examples 1-10.

The applicant's attention is drawn to the fact that claims, or parts of claims, relating to inventions in respect of which no international search report has been established need not be the subject of an international preliminary examination (Rule 66.1(e) PCT). The applicant is advised that the EPO policy when acting as an International Preliminary Examining Authority is normally not to carry out a preliminary examination on matter which has not been searched. This is the case irrespective of whether or not the claims are amended following receipt of the search report or during any Chapter II procedure.

FURTHER INFORMATION CONTINUED FROM PCT/ISA/ 210

1. Claims: 1-101, 119-128, 129-132 partly, 133-151, 153-162

Isolated terpene synthases having a region with 20% or greater sequence identity to residues 265 to 535 of SEQ.ID.NO:2 (tobacco 5-epi-aristolochene synthase) and having an ordered arrangement of R-groups at active-center alpha-carbons other than those characterized in Tables 7-9; fusion proteins comprising said terpene synthases; methods for making said terpene synthases; nucleic acids encoding said terpene synthases; host cells containing said nucleic acids; transgenic plants containing said nucleic acids and transgenic animal cell cultures containing said nucleic acids.

2. Claims: 102, 129 partly, 130 partly, 152 partly

An isolated synthase having 40% or greater sequence identity to residues 343 to 612 of SEQ.ID.NO: 20 (pinene synthase) having an arrangement of amino acid residues at active site positions other than a range of specified ordered arrangements (see page 290 description); method for synthesizing said synthase and an isolated nucleic acid encoding said synthase.

3. Claims: 103, 152 partly

An isolated synthase having 40% or greater sequence identity to residues 316 to 586 of SEQ.ID.NO: 22 (spearmint limonene synthase) having an arrangement of amino acid residues at active site positions other than a range of specified ordered arrangements (see page 292 description); method for synthesizing said synthase and an isolated nucleic acid encoding said synthase.

4. Claims: 104, 152 partly

An isolated synthase having 40% or greater sequence identity to residues 352 to 622 of SEQ.ID.NO: 58 (grand fir limonene synthase) having an arrangement of amino acid residues at active site positions other than a range of specified ordered arrangements (see page 294 description); method for synthesizing said synthase and an isolated nucleic acid encoding said synthase.

5. Claims: 105, 152 partly

An isolated synthase having 40% or greater sequence identity to residues 272 to 540 of SEQ.ID.NO: 33 (cotton delta catadinene synthase) having an arrangement of amino acid residues at active site positions other than a range of specified ordered arrangements (see page 296 description); method for synthesizing said synthase and an isolated

FURTHER INFORMATION CONTINUED FROM PCT/ISA/ 210

nucleic acid encoding said synthase.

6. Claims: 106, 152 partly

An isolated synthase having 40% or greater sequence identity to residues 319 to 571 of SEQ.ID.NO: 42 (castor bean casbene synthase) having an arrangement of amino acid residues at active site positions other than a range of specified ordered arrangements (see page 298 description); method for synthesizing said synthase and an isolated nucleic acid encoding said synthase.

7. Claims: 107, 131 partly, 132 partly, 152 partly

An isolated synthase having 40% or greater sequence identity to residues 579 to 847 of SEQ.ID.NO: 44 (yew taxadiene synthase) having an arrangement of amino acid residues at active site positions other than a range of specified ordered arrangements (see page 300 description); method for synthesizing said synthase and an isolated nucleic acid encoding said synthase.

8. Claims: 108, 152 partly

An isolated synthase having 40% or greater sequence identity to residues 495 to 767 of SEQ.ID.NO: 46 (grand fir E-alpha bisabolene synthase) having an arrangement of amino acid residues at active site positions other than a range of specified ordered arrangements (see page 302 description); method for synthesizing said synthase and an isolated nucleic acid encoding said synthase.

9. Claims: 109, 152 partly

An isolated synthase having 40% or greater sequence identity to residues 295 to 564 of SEQ.ID.NO: 48 (grand fir delta selinene synthase) having an arrangement of amino acid residues at active site positions other than a range of specified ordered arrangements (see page 304 description); method for synthesizing said synthase and an isolated nucleic acid encoding said synthase.

10. Claims: 110, 152 partly

An isolated synthase having 40% or greater sequence identity to residues 307 to 578 of SEQ.ID.NO: 50 (grand fir gamma humulene synthase) having an arrangement of amino acid residues at active site positions other than a range of specified ordered arrangements (see page 306 description); method for synthesizing said synthase and an isolated

FURTHER INFORMATION CONTINUED FROM PCT/ISA/ 210

nucleic acid encoding said synthase.

11. Claims: 111, 152 partly

An isolated synthase having 40% or greater sequence identity to residues 264 to 533 of SEQ.ID.NO: 52 (tomato germacrene synthase) having an arrangement of amino acid residues at active site positions other than a range of specified ordered arrangements (see page 308 description); method for synthesizing said synthase and an isolated nucleic acid encoding said synthase.

12. Claims: 112, 152 partly

An isolated synthase having 40% or greater sequence identity to residues 585 to 853 of SEQ.ID.NO: 56 (grand fir abiatadiene synthase) having an arrangement of amino acid residues at active site positions other than a range of specified ordered arrangements (see page 310 description); method for synthesizing said synthase and an isolated nucleic acid encoding said synthase.

13. Claims: 113, 152 partly

An isolated synthase having 40% or greater sequence identity to residues 307 to 574 of SEQ.ID.NO: 54 (sage +sabinene synthase) having an arrangement of amino acid residues at active site positions other than a range of specified ordered arrangements (see page 312 description); method for synthesizing said synthase and an isolated nucleic acid encoding said synthase.

14. Claims: 114, 152 partly

An isolated synthase having 40% or greater sequence identity to residues 309 to 577 of SEQ.ID.NO: 24 (sage 1,8-cineole synthase) having an arrangement of amino acid residues at active site positions other than a range of specified ordered arrangements (see page 314 description); method for synthesizing said synthase and an isolated nucleic acid encoding said synthase.

15. Claims: 115, 152 partly

An isolated synthase having 40% or greater sequence identity to residues 315 to 584 of SEQ.ID.NO: 26 (sage bornyl diphosphate synthase) having an arrangement of amino acid residues at active site positions other than a range of specified ordered arrangements (see page 316 description); method for synthesizing said synthase and an isolated

FURTHER INFORMATION CONTINUED FROM PCT/ISA/ 210

nucleic acid encoding said synthase.

16. Claims: 116, 152 partly

An isolated synthase having 40% or greater sequence identity to residues 265 to 536 of SEQ.ID.NO: 28 (mint E-b-farnesene synthase) having an arrangement of amino acid residues at active site positions other than a range of specified ordered arrangements (see page 318 description); method for synthesizing said synthase and an isolated nucleic acid encoding said synthase.

17. Claims: 117, 152 partly

An isolated synthase having 40% or greater sequence identity to residues 342 to 612 of SEQ.ID.NO: 30 (grand fir myrcene synthase) having an arrangement of amino acid residues at active site positions other than a range of specified ordered arrangements (see page 320 description); method for synthesizing said synthase and an isolated nucleic acid encoding said synthase.

18. Claims: 118, 152 partly

An isolated synthase having 40% or greater sequence identity to residues 307 to 541 of SEQ.ID.NO: 32 (potato vetaspiradiene synthase) having an arrangement of amino acid residues at active site positions other than a range of specified ordered arrangements (see page 322 description); method for synthesizing said synthase and an isolated nucleic acid encoding said synthase.

INTERNATIONAL SEARCH REPORT

Information on patent family members

International Application No

PCT/US 99/21419

| Patent document cited in search report | Publication date | Patent family member(s) | Publication date |
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For two-letter codes and other abbreviations, refer to the "Guidance Notes on Codes and Abbreviations" appearing at the beginning of each regular issue of the PCT Gazette.

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(72) Inventors: CHAPPELL, Joseph; 1808 Bimini Road, Lexington, KY 40502 (US). MANNA, Kathleen, R.; 1010 Brookstone Court, Georgetown, IN 47122 (US). NOEL, Joseph, P.; 7280 Park Village Road, San Diego, CA 92129 (US). STARKS, Courtney, M.; University of California, 9500 Gilman Drive, Mail Code 0204, La Jolla, CA 92093-0204 (US).

(74) Agent: LUNDQUIST, Ronald, C.; Fish & Richardson P.C., P.A., Suite 3300, 60 South Sixth Street, Minneapolis, MN 55402 (US).

(54) Title: TERPENE SYNTHASES

(57) Abstract: Novel synthases and the corresponding nucleic acids encoding such synthases are disclosed herein. Such synthases possess an active site pocket that includes key amino acid residues that are modified to generate desired terpenoid reaction intermediates and products. Synthase modifications are designed based on, e.g., the three-dimensional coordinates of tobacco 5-cpi-aristolochene synthase, with or without a substrate bound in the active site.

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TERPENE SYNTHASES

Cross Reference to Related Application

This application claims the benefit of provisional application 60/100,993 filed September 18, 1998; provisional application 60/130,628 filed April 22, 1999; and provisional application 60/150,262 filed August 23, 1999.

This work was supported, in part, with funding from Federal agencies. Therefore, the United States Federal Government may have certain rights in the invention.

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Background of the Invention

Isoprenoid compounds are organic molecules produced by a wide range of organisms (e.g., plants, bacteria, fungi, etc). To date, over 23,000 individual isoprenoid molecules have been characterized with tens to hundreds of new structures identified each year. These molecules can fulfill a variety of roles. For example, monoterpenes can be used as fragrances and flavors. Sesquiterpenes and diterpenes can serve as pheromones, defensive agents, visual pigments, antitumor drugs, and components of signal transduction pathways. Triterpenes can serve important functions as membrane constituents and precursors of steroid hormones and bile acids. Polyprenols function as photoreceptive agents and cofactor side chains, and can also exist as natural polymers.

The diverse molecular compounds produced by the isoprenoid pathway are created from diphosphate esters of monounsaturated isoprene units. Isoprenes are added together in multiples of 2, 3, or 4 by prenyl transferases to make C_{10} , C_{15} , and C_{20} units, respectively. The C_{10} , C_{15} , and C_{20} molecules, named geranyl diphosphate (GPP), farnesyl diphosphate (FPP), and geranylgeranyl diphosphate (GGPP), respectively, serve as substrates for terpene synthases.

Terpene synthases catalyze the production of isoprenoid compounds via one of the most complex reactions known in chemistry or biology. In general, terpene synthases are moderately sized enzymes having molecular weights of about 40 to 100 kD. As an enzyme, terpene synthases can be classified as having low to moderate turnover rates coupled with exquisite reaction specificity and preservation

of chirality. Turnover comprises binding of substrate to the enzyme, establishment of substrate conformation, conversion of substrate to product and product release.

Reactions can be performed in vitro in aqueous solvents, typically require magnesium ions as cofactors, and the resulting products, which are often highly hydrophobic, can be recovered by partitioning into an organic solvent.

Terpene synthase genes are found in a variety of organisms including bacteria, fungi and plants. Swapping regions approximating exons between different terpene synthases has identified functional domains responsible for terminal enzymatic steps. For example, work performed on 5-epi-aristolochene synthase (TEAS) from *Nicotiana tabacum* (tobacco) and *Hyoscyamus muticus* vetispiradiene synthase (HVS) from henbane revealed that exon 4 and exon 6, respectively, were responsible for reaction product specificity. Combining functional domains resulted in novel enzymes capable of synthesizing new reaction products (U.S. Patent 5,824,774).

Studies have led to proposed reaction mechanisms for isoprenoid production; see, e.g., Cane et al., 1985, *Bioorg. Chem.*, 13:246-265; Wheeler and Croteau, 1987, *Proc. Natl. Acad. Sci. USA*, 84:4856-4859; and Pyun et al., 1994, *Arch. Biochem. Biophys.*, 308:488-496. The studies used substrate analogs and suicide inhibitors (Croteau, 1994, *Arch. Biochem. Biophys.*, 251:777-782; Cane et al., 1995, *Biochemistry*, 34:2471-2479; and Croteau et al., 1993, *Arch. Biochem. Biophys.*, 307:397-404), as well as chemical-modifying reagents and site-directed mutagenesis in efforts to identify amino acids essential for catalysis (Cane et al., 1995, *Biochemistry*, 34:2480-2488; Rajaonarivony et al., 1992, *Arch. Biochem. Biophys.*, 296:49-57; and Rajaonarivony et al., 1992, *Arch. Biochem. Biophys.*, 299:77-82). However, these studies have resulted in limited success in defining the active site due to inherent limitations with these techniques.

Summary of the Invention

The invention describes a method of identifying alpha-carbon atoms found in the active site of a terpene synthase and describes these atoms in three-dimensional space as well as the spatial relationships among them. The present invention also describes R-groups associated with such alpha-carbons and methods of altering these R-groups in order to create novel terpene synthases capable of generating novel reaction products.

Until the invention taught in this present application, the active site of synthase proteins, the amino acid residues located therein, the amino acid residues involved in catalysis, and the configuration of α -carbons and R-groups within the

active site have not been known. The current invention now teaches the structure of synthases, as well as provides the means of making and using the information obtained therefrom to develop and produce new and novel synthases having new and novel synthetic capabilities. The data generated using the methods described
5 herein are useful for creation and production of synthase mutants that can use a variety of isoprenoid substrates and produce a variety of isoprenoid products.

In one embodiment, the invention features an isolated terpene synthase having about 20% or greater sequence identity to residues 265 to 535 of SEQ ID NO: 2. Such a synthase comprises nine α -carbons having interatomic
10 distances in Angstroms between the α -carbons that are ± 2.3 Angstroms of the interatomic distances shown in Table 6. The center point of each α -carbon is positioned within a sphere having a radius of 2.3 Angstroms. The center point of each such sphere has the structural coordinates given in Table 5. Each α -carbon has an associated R-group, and the synthase has an ordered arrangement of R-
15 groups associated with each alpha-carbon other than the ordered arrangements of R-groups shown in Table 9. The synthase can have about 25% or greater sequence identity to residues 265 to 535 of SEQ ID 2, or about 35% or greater sequence identity to residues 265 to 535 of SEQ ID 2. Such a synthase can catalyse the formation of a terpenoid product from a monoterpene substrate, a sesquiterpene
20 substrate, or a diterpene substrate. The product can be a cyclic terpenoid hydrocarbon or an acyclic terpenoid hydrocarbon. Either type of product can be hydroxylated or non-hydroxylated. The R-group associated with α -carbon 1 can be selected from one of the following groups: the group consisting of Cys, Ser, and Thr, the group consisting of Phe, Tyr and Trp, the group consisting of Pro, Gly, and Ala,
25 the group consisting of Glu and Asp, the group consisting of Met, Ile, Val and Leu, the group consisting of Arg and Lys, and the group consisting of Gln, Asn and His. R-groups associated with α -carbons 2 to 9 can be any amino acid except those having the ordered arrangements of Table 9. Similarly, the R-group associated with each of α -carbons 2-9 can be selected independently from the group consisting of
30 Cys, Ser and Thr, the group consisting of Phe, Tyr and Trp, the group consisting of Pro, Gly, and Ala, the group consisting of Glu and Asp, the group consisting of Met, Ile, Val and Leu, the group consisting of Arg and Lys, and the group consisting of Gln, Asn and His. In these embodiments, R-groups associated with the remaining eight α -carbons except those having the ordered arrangements of Table 9.

35 In some embodiments, the ordered arrangement of R-groups associated with α -carbons 1 to 9 is Trp, Ile, Thr, Thr, Tyr, Leu, Cys, Thr and Phe, respectively, Ser, Ile, Thr, Thr, Tyr, Leu, Cys, Thr and Tyr, respectively, Trp, Ile, Thr,

Thr, Tyr, Leu, Trp, Thr and Tyr, respectively, Ser, Ile, Thr, Thr, Tyr, Leu, Trp, Thr and Tyr, respectively, or Glu, Ile, Thr, Thr, Tyr, Leu, Cys, Thr and Tyr, respectively.

The invention also features a terpene synthase made by aligning the primary amino acid sequence of a preselected terpene synthase polypeptide to the amino acid sequence of residues 265 to 535 of SEQ ID NO: 2, mutating a nucleic acid encoding the preselected polypeptide at one or more codons for nine amino acid residues in a region of the polypeptide primary amino acid sequence having about 20% or greater sequence identity to residues 265 to 535 of SEQ ID NO: 2, the nine residues in the polypeptide aligning with residues 273, 294, 402, 403, 404, 407, 440, 519 and 520 of SEQ ID NO: 2; and expressing the mutated nucleic acid so that a mutated terpene synthase is made.

The invention also features an isolated terpene synthase having about 20% or greater sequence identity to residues 265 to 535 of SEQ ID NO: 2, the synthase comprising sixteen α -carbons having interatomic distances in Angstroms between the α -carbons that are ± 2.3 Angstroms of the interatomic distances given in Table 4. The center point of each α -carbon is positioned within a sphere having a radius of 2.3 Angstroms. The center point of each of the spheres has the structural coordinates given in Table 3. Each α -carbon has an associated R-group, and the synthase has an ordered arrangement of R-groups other than the ordered arrangements of R-groups given in Table 8. The synthase can have about 25% or greater sequence identity to residues 265 to 535 of SEQ ID NO: 2, or about 35% or greater sequence identity to residues 265 to 535 of SEQ ID NO: 2. The synthase can catalyse the formation of a terpenoid product from a monoterpene substrate, a sesquiterpene substrate, or a diterpene substrate. The product can be, for example, a cyclic terpenoid hydrocarbon. The ordered arrangement of R-groups in the synthase associated with α -carbons 1 to 16 can be Cys, Trp, Ile, Ile, Ser, Thr, Thr, Tyr, Leu, Cys, Val, Thr, Tyr, Asp, Phe and Thr, respectively.

The invention also features an isolated terpene synthase having about 20% or greater sequence identity to residues 265 to 535 of SEQ ID NO: 2, the synthase comprising nineteen α -carbons having interatomic distances in Angstroms between the α -carbons that are ± 2.3 Angstroms of the interatomic distances given in Table 2. The center point of each α -carbon is positioned within a sphere having a radius of 2.3 Angstroms. The center points of each sphere have the structural coordinates given in Table 1. Each α -carbon has an associated R-group, and the synthase has an ordered arrangement of the R-groups other than the ordered arrangements of R-groups given in Table 7. The synthase can have about 25% or greater sequence identity to residues 265 to 535 of SEQ ID NO: 2, or about 35% or

greater sequence identity to residues 265 to 535 of SEQ ID NO: 2. The synthase can catalyse the formation of a terpenoid product from a monoterpene substrate, a sesquiterpene substrate, or a diterpene substrate. The product can be, for example, a cyclic terpenoid hydrocarbon.

5 The invention also features an isolated protein comprising a first domain having an amino terminal end and a carboxyl terminal end. The first domain comprises amino acids that align structurally in three-dimensional space with a glycosyl hydrolase catalytic core, the glycosyl hydrolase catalytic core selected from the group consisting of amino acids 36 to 230 of glucoamylase protein databank (PDB) code 3GLY of *Aspergillus awamori* and amino acids 36 to 230 of endoglucanase CelD PDB code 1CLC. The isolated protein also comprises a second domain having an amino terminal end and carboxyl terminal end. The second domain comprises amino acids that align structurally in three-dimensional space with avian FPP synthase. The carboxyl terminal end of the first domain is linked to the amino terminal end of the second domain. The second domain has about 20% or greater sequence identity to residues 265 to 535 of SEQ ID NO: 2, and comprises nine α -carbons having interatomic distances in Angstroms between the α -carbons that are ± 2.3 Angstroms of the interatomic distances given in Table 6. The center point of each α -carbon is positioned within a sphere having a radius of 2.3 Angstroms, the center point of each sphere having the structural coordinates given in Table 5. Each α -carbon has an associated R-group, and the synthase has an ordered arrangement of R-groups other than the ordered arrangements of R-groups given in Table 9. The protein can have about 25% or greater sequence identity to SEQ ID NO: 2, or about 35% or greater sequence identity to SEQ ID NO: 2. The synthase can catalyse the formation of a terpenoid product from a monoterpene substrate, a sesquiterpene substrate, or a diterpene substrate. The product can be, for example, a cyclic terpenoid hydrocarbon.

 The invention also features an isolated synthase having a region with about 40% or greater sequence identity to residues 343 to 606 of SEQ ID NO: 20, wherein one or more amino acid residues of the synthase that align with amino acid residues at positions 348, 351, 372, 375, 376, 454, 479, 480, 481, 482, 485, 519, 523, 597, 600, 601, 605, 607 and 608 of SEQ ID NO: 20 are residues other than amino acids Y, L, C, I, T, Y, S, C, G, H, S, L, G, F, G, Y, D, Y and S, respectively. In some embodiments, the sequence identity can be about 20% or greater, 25% or greater, or 35% or greater. In some embodiments, one or more of the ordered arrangements of residues as given in Table 7 are not found in such a synthase.

The invention also features an isolated synthase having a region with about 40% or greater sequence identity to residues 316 to 586 of SEQ ID NO: 22, wherein one or more amino acid residues of the synthase that align with amino acid residues at positions 321, 324, 345, 348, 349, 427, 452, 453, 454, 455, 458, 492, 496, 569, 572, 573, 577, 579 and 580 of SEQ ID NO: 22 are residues other than amino acids C, W, N, I, T, Y, S, I, S, G, M, L, D, A, M, Y, D, H and G, respectively. In some embodiments, the sequence identity can be about 20% or greater, 25% or greater, or 35% or greater. In some embodiments, one or more ordered arrangements of residues as given in Table 7 are not found in such a synthase.

10 The invention also features an isolated synthase having a region with about 40% or greater sequence identity to residues 352 to 622 of SEQ ID NO: 58, wherein one or more amino acid residues of the synthase that align with amino acid residues at positions 357, 360, 381, 384, 385, 463, 487, 488, 489, 490, 493, 528, 532, 606, 609, 610, 614, 616 and 617 of SEQ ID NO: 58 are residues other than amino acids Y, M, C, V, T, F, V, S, S, G, I, L, G, F, V, Y, D, Y and T, respectively. In some embodiments, the sequence identity can be about 20% or greater, 25% or greater, or 35% or greater. In some embodiments, one or more of the ordered arrangements of residues as given in Table 7 are not found in such a synthase.

20 The invention also features an isolated synthase having a region with about 40% or greater sequence identity to amino acid residues 272 to 540 encoded by SEQ ID NO: 33, wherein one or more amino acid residues of the synthase that align with amino acid residues at positions 277, 280, 301, 304, 305, 383, 408, 409, 410, 411, 414, 448, 452, 524, 527, 528, 532, 534 and 535 encoded by SEQ ID NOS: 33 are residues other than amino acids G, W, I, A, S, Y, T, S, G, Y, L, C, D, M, L, Y, D, Y and T, respectively. In some embodiments, the sequence identity can be about 20% or greater, 25% or greater, or 35% or greater. In some embodiments, one or more of the ordered arrangements of residues as given in Table 7 are not found in such a synthase.

30 The invention also features an isolated synthase having a region with about 40% or greater sequence identity to residues 319 to 571 of SEQ ID NO: 42, wherein one or more amino acid residues of the synthase that align with amino acid residues at positions 324, 327, 348, 351, 352, 430, 455, 456, 457, 458, 461, 495, 499, 571, 574, 575, 579, 581 and 582 of SEQ ID NO: 42 are residues other than amino acids I, W, V, I, S, Y, T, T, G, L, V, I, N, T, S, Y, D, Y, and T, respectively. In some embodiments, the sequence identity can be about 20% or greater, 25% or greater, or 35% or greater. In some embodiments, one or more of the ordered arrangements of residues as given in Table 7 are not found in such a synthase.

The invention also features an isolated synthase having a region with about 40% or greater sequence identity to residues 579 to 847 of SEQ ID NO: 44, wherein one or more amino acid residues of the synthase that align with amino acid residues at positions 584, 587, 606, 609, 610, 688, 713, 714, 715, 716, 719, 753, 757, 831, 834, 835, 839, 841 and 842 of SEQ ID NO: 44 are residues other than amino acids V, S, G, Q, V, Y, S, V, G, L, C, W, N, V, F, Y, D, Y and G, respectively. In some embodiments, the sequence identity can be about 20% or greater, 25% or greater, or 35% or greater. In some embodiments, one or more of the ordered arrangements of residues as given in Table 7 are not found in such a synthase.

The invention also features an isolated synthase having a region with about 40% or greater sequence identity to residues 495 to 767 of SEQ ID NO: 46, wherein one or more amino acid residues of the synthase that align with amino acid residues at positions 500, 503, 524, 527, 528, 606, 631, 632, 633, 634, 637, 674, 678, 751, 754, 755, 759, 761 and 762 of SEQ ID NO: 46 are residues other than amino acids F, L, A, Q, T, Y, S, I, G, Q, L, S, D, T, I, F, D, F and G, respectively. In some embodiments, the sequence identity can be about 20% or greater, 25% or greater, or 35% or greater. In some embodiments, one or more of the ordered arrangements of residues as given in Table 7 are not found in such a synthase.

The invention also features an isolated synthase having a region with about 40% or greater sequence identity to residues 295 to 564 of SEQ ID NO: 48, wherein one or more amino acid residues of the synthase that align with amino acid residues at positions 300, 303, 324, 327, 328, 406, 431, 432, 433, 434, 437, 471, 475, 548, 551, 552, 556, 558 and 559 of SEQ ID NO: 48 are residues other than amino acids Y, W, A, C, T, Y, S, S, G, M, L, G, D, L, I, Y, D, L and Y, respectively. In some embodiments, the sequence identity can be about 20% or greater, 25% or greater, or 35% or greater. In some embodiments, one or more of the ordered arrangements of residues as given in Table 7 are not found in such a synthase.

The invention also features an isolated synthase having a region with about 40% or greater sequence identity to residues 307 to 578 of SEQ ID NO: 50, wherein one or more amino acid residues of the synthase that align with amino acid residues at positions 312, 315, 336, 339, 340, 419, 444, 445, 446, 447, 450, 484, 488, 562, 565, 566, 570, 572 and 573 of SEQ ID NO: 50 are residues other than amino acids F, W, A, M, T, Y, N, T, G, M, L, S, D, I, M, Y, D, F and S, respectively. In some embodiments, the sequence identity can be about 20% or greater, 25% or greater, or 35% or greater. In some embodiments, one or more of the ordered arrangements of residues as given in Table 7 are not found in such a synthase.

The invention also features an isolated synthase having a region with about 40% or greater sequence identity to residues 264 to 533 of SEQ ID NO: 52, wherein one or more amino acid residues of the synthase that align with amino acid residues at positions 269, 272, 293, 296, 297, 375, 401, 402, 403, 404, 407, 441, 445, 517, 520, 521, 525, 527 and 528 of SEQ ID NO: 52 are residues other than amino acids C, W, L, T, S, Y, S, A, G, Y, I, A, N, A, L, Y, D, Y and S, respectively. In some embodiments, the sequence identity can be about 20% or greater, 25% or greater, or 35% or greater. In some embodiments, one or more of the ordered arrangements of residues as given in Table 7 are not found in such a synthase.

The invention also features an isolated synthase having a region with about 40% or greater sequence identity to residues 585 to 853 of SEQ ID NO: 56, wherein one or more amino acid residues of the synthase that align with amino acid residues at positions 590, 593, 614, 617, 618, 696, 721, 722, 723, 724, 727, 761, 765, 837, 840, 841, 845, 847 and 848 of SEQ ID NO: 56 are residues other than amino acids I, S, S, T, V, Y, S, I, A, L, V, G, N, M, F, Y, D, L and T, respectively. In some embodiments, the sequence identity can be about 20% or greater, 25% or greater, or 35% or greater. In some embodiments, one or more of the ordered arrangements of residues as given in Table 7 are not found in such a synthase.

The invention also features an isolated synthase having a region with about 40% or greater sequence identity to residues 307 to 574 of SEQ ID NO: 54, wherein one or more amino acid residues of the synthase that align with amino acid residues at positions 312, 315, 336, 339, 340, 418, 443, 444, 445, 446, 449, 483, 487, 560, 563, 564, 566, 568 and 569 of SEQ ID NO: 54 are residues other than amino acids C, W, I, I, T, Y, S, I, S, A, I, L, D, A, I, Y, D, D and G, respectively. In some embodiments, the sequence identity can be about 20% or greater, 25% or greater, or 35% or greater. In some embodiments, one or more of the ordered arrangements of residues as given in Table 7 are not found in such a synthase.

The invention also features an isolated synthase having a region with about 40% or greater sequence identity to residues 309 to 577 of SEQ ID NO: 24, wherein one or more amino acid residues of the synthase that align with amino acid residues at positions 314, 317, 338, 341, 342, 420, 446, 447, 448, 449, 452, 485, 489, 560, 563, 564, 569, 571 and 572 of SEQ ID NO: 24 are residues other than amino acids C, W, N, V, T, Y, I, G, G, I, L, L, D, A, I, Y, D, F and G, respectively. In some embodiments, the sequence identity can be about 20% or greater, 25% or greater, or 35% or greater. In some embodiments, one or more of the ordered arrangements of residues as given in Table 7 are not found in such a synthase.

The invention also features an isolated synthase having a region with about 40% or greater sequence identity to residues 315 to 584 of SEQ ID NO: 26, wherein one or more amino acid residues of the synthase that align with amino acid residues at positions 320, 323, 344, 347, 348, 426, 451, 452, 453, 454, 457, 492, 496, 568, 571, 572, 576, 578 and 579 of SEQ ID NO: 26 are residues other than amino acids S, W, I, A, T, Y, S, V, A, S, I, L, D, A, I, Y, D, F, and G, respectively. In some embodiments, the sequence identity can be about 20% or greater, 25% or greater, or 35% or greater. In some embodiments, one or more of the ordered arrangements of residues as given in Table 7 are not found in such a synthase.

The invention also features an isolated synthase having a region with about 40% or greater sequence identity to residues 265 to 536 of SEQ ID NO: 28, wherein one or more amino acid residues of the synthase that align with amino acid residues at positions 270, 273, 294, 297, 298, 376, 401, 402, 403, 404, 407, 440, 444, 518, 521, 522, 528, 530 and 531 of SEQ ID NO: 28 are residues other than amino acids A, W, V, C, G, F, T, S, C, I, M, G, N, C, S, Y, D, Y and S, respectively. In some embodiments, the sequence identity can be about 20% or greater, 25% or greater, or 35% or greater. In some embodiments, one or more of the ordered arrangements of residues as given in Table 7 are not found in such a synthase.

The invention also features an isolated synthase having a region with about 40% or greater sequence identity to residues 342 to 612 of SEQ ID NO: 30, wherein one or more amino acid residues of the synthase that align with amino acid residues at positions 347, 350, 371, 374, 375, 453, 478, 479, 480, 481, 483, 518, 522, 596, 599, 600, 604, 606 and 607 of SEQ ID NO: 30 are residues other than amino acids F, L, C, V, T, Y, S, S, A, Y, V, L, G, L, L, Y, D, F and S, respectively. In some embodiments, the sequence identity can be about 20% or greater, 25% or greater, or 35% or greater. In some embodiments, one or more of the ordered arrangements of residues as given in Table 7 are not found in such a synthase.

The invention also features an isolated synthase having a region with about 40% or greater sequence identity to residues 273 to 541 of SEQ ID NO: 32, wherein one or more amino acid residues of the synthase that align with amino acid residues at positions 278, 281, 302, 305, 306, 384, 409, 410, 411, 412, 415, 448, 452, 524, 527, 528, 533, 535 and 536 of SEQ ID NO: 32 are residues other than amino acids C, W, I, I, S, Y, T, S, T, Y, L, C, D, I, T, Y, D, Y and T, respectively. In some embodiments, the sequence identity can be about 20% or greater, 25% or greater, or 35% or greater. In some embodiments, one or more ordered arrangements of residues as given in Table 7 are not found in such a synthase.

The invention also features a method for making a terpene synthase, comprising identifying, in a preselected polypeptide having a region with 20% or greater sequence identity to residues 265 to 535 of SEQ ID NO: 2, nine amino acid residues whose α -carbons have interatomic distances in Angstroms between the α -carbons that are ± 2.3 Angstroms of the interatomic distances given in Table 6. The center point of each α -carbon is positioned within a sphere having a radius of 2.3 Angstroms. The center point of each sphere has the structural coordinates given in Table 5. The method then comprises synthesizing a polypeptide that is modified from the preselected polypeptide. The modified polypeptide has one or more R-groups associated with the nine α -carbons other than the R-groups associated with the α -carbons in the preselected polypeptide. The synthesizing step can comprise the formation of a nucleic acid encoding the preselected polypeptide in which the coding sequence for one or more amino acids corresponding to the nine α -carbons is replaced by a coding sequence that codes for an amino acid different from the amino acid present in the preselected polypeptide. The preselected polypeptide can be, for example, any one of the polypeptides given in SEQ ID NOS: 2, 4, 6, 8, 10, 12, 20, 22, 24, 26, 28, 30, 32, 34-40, 42, 44, 46, 48, 50, 52, 54, 56, or 58.

The invention also features a method of using a terpene synthase, comprising identifying, in a preselected polypeptide having a region with 20% or greater sequence identity to residues 265 to 535 of SEQ ID NO: 2, amino acid residues at nine positions that align with amino acid residues 273, 294, 402, 403, 404, 407, 440, 519 and 520 of SEQ ID NO: 2; and synthesizing a polypeptide that is modified from the preselected polypeptide. The novel polypeptide is modified by having amino acid residues at one or more of the nine positions other than the amino acid residues present in the preselected polypeptide. In some embodiments, the identifying step can comprise identifying sixteen amino acid residues in the preselected polypeptide that align with amino acid residues 270, 273, 294, 297, 298, 402, 403, 404, 407, 440, 516, 519, 520, 525, 527 and 528 of SEQ ID NO: 2, and the synthesizing step can comprise synthesizing a polypeptide that is modified from the preselected polypeptide, the modified polypeptide having amino acid residues at one or more of the sixteen positions other than the amino acid residues present in the preselected polypeptide. In some embodiments, the identifying step can comprise identifying nineteen amino acid residues in the preselected polypeptide that align with amino acid residues 270, 273, 294, 297, 298, 376, 401, 402, 403, 404, 407, 440, 444, 516, 519, 520, 525, 527 and 528 of SEQ ID NO: 2, and the synthesizing step can comprise synthesizing a polypeptide that is modified from the preselected polypeptide, the modified polypeptide having amino acid residues at one or more of

the nineteen positions other than the amino acid residues present in the preselected polypeptide. The synthesizing step can comprise the formation of a nucleic acid encoding the preselected polypeptide in which the coding sequence in the nucleic acid coding for one or more of the identified amino acid residues is replaced by a coding sequence that encodes an amino acid different from the amino acid present in the preselected polypeptide. The preselected polypeptide can be, for example, any one of the polypeptides given in SEQ ID NOS: 2, 4, 6, 8, 10, 12, 20, 22, 24, 26, 28, 30, 32, 34-40, 42, 44, 46, 48, 50, 52, 54, 56, or 58. The method can further comprise: contacting the modified polypeptide with an isoprenoid substrate under conditions effective for the compound to bind the polypeptide; and measuring the ability of the modified polypeptide to catalyze the formation of a reaction product from the isoprenoid substrate. The isoprenoid substrate can be a monoterpene, a sesquiterpene, or a diterpene.

The invention also features a method of making a terpene synthase, comprising creating a population of nucleic acid molecules that encode polypeptides, the population having members that differ from one another at one or more of nine codons specifying amino acids of a preselected terpene synthase having a region with about 20% or greater sequence identity to residues 265 to 535 of SEQ ID NO: 2, α -carbons of the nine amino acids having interatomic distances in Angstroms between the α -carbons that are ± 2.3 Angstroms of the interatomic distances given in Table 6. The center point of each α -carbon is positioned within a sphere having a radius of 2.3 Angstroms, and the center point of each sphere has the structural coordinates given in Table 5. In some embodiments, the codons specify amino acids as described in Tables 1-2 or 3-4 of a preselected terpene synthase. A portion, or all, of the nucleic acid population is expressed so that a population of polypeptides is made. At least one member of the population of polypeptides is a mutant terpene synthase. The expressing step can comprise in vitro transcription and in vitro translation of the nucleic acid population. In some embodiments, the expressing step comprises cloning members of the nucleic acid population into an expression vector; introducing the expression vector into host cells and expressing the cloned nucleic acid population members in the host cells so that the population of polypeptides is made. The preselected terpene synthase polypeptide can be a monoterpene synthase, a sesquiterpene synthase, or a diterpene synthase. The host cells can be prokaryotic cells or eukaryotic cells, including, without limitation, bacterial cells, fungal cells, and animal cells, e.g., mammalian cells or insect cells. The host cells can also be plant cells, e.g., a cell from a Graminaceae plant, a cell from a

Legumineae plant, a cell from a Solanaceae plant, a cell from a Brassicaceae plant or a cell from a Conifereae plant.

The invention also features a nucleic acid encoding a synthase as described herein, and a host cell containing such a nucleic acid. The invention also
5 features a transgenic plant containing such a nucleic acid, or a transgenic animal cell culture containing such a nucleic acid.

In some embodiments, a synthase polypeptide of the invention comprises a domain that contains an active site comprised of nine α -carbon atoms having the coordinates of Table 5, and interatomic distances between the α -carbons
10 ± 2.3 angstroms of the distances given in Table 6. The α -carbon atoms align structurally in three dimensional space in the presence or absence of bound substrate or substrate analogue, with avian FPP synthase. In another embodiment, a synthase of this invention comprises the following: (i) a first domain containing amino acid residues that align in three-dimensional space (in solution or crystal form,
15 and either having a bound or unbound substrate) with a glycosyl hydrolase catalytic core selected from the group consisting of (a) amino acids 36-230 of glycosyl hydrolase (PDB code 3GLY) of *Aspergillus awamori*, and (b) amino acids 36-230 of endoglucanase CellB (PDB code 1CLC), and (ii) a second domain that aligns structurally in three dimensional space with or without substrate or substrate
20 analogues bound in the active site with avian FPP synthase. The second domain contains an active site comprised of nine, sixteen or nineteen α -carbon atoms having the structural coordinates and interatomic distances of Tables 1-2, 3-4 or 5-6. These α -carbon atoms have R-groups attached thereto that can interact, either directly or indirectly, with an isoprenoid substrate.

25 The invention also features a method for generating mutant terpene synthases possessing catalytic activity. The method comprises the steps of (a) providing a crystallographic model of a preselected catalytically active terpene synthase having an active site, and (b) using the model to design a terpene synthase having at least one altered R-group in the active site relative to the preselected
30 synthase. The invention also features terpene synthases having altered substrate specificity, methods of making the same, and procedures for generating three-dimensional structures thereof.

Although methods and materials similar or equivalent to those described herein can be used to practice the invention, suitable methods and
35 materials are described below. All publications, patent applications, patents and other references mentioned herein are incorporated by reference in their entirety.

Other aspects, embodiments, advantages, and features of the present invention will become apparent from the specification.

Brief Description of Drawings

5 Figure 1. Schematic representation of tobacco 5-epi-aristolochene synthase (TEAS) with bound farnesyl hydroxyphosphonate (FHP), prepared using the RIBBONS software program of Carson, M. and Bugg, C., J. Mol. Graphics 4:121 (1986).

10 Figure 2. Structure of twenty natural amino acids showing α -carbons and associated R-groups.

 Figure 3. Autoradiogram of an argention thin-layer chromatogram of terpenoid hydrocarbon products made by TEAS and mutant TEAS enzymes using GGPP as a substrate. DM: W273S/C440W mutant TEAS enzyme.

15 Figure 4. Autoradiogram of an argention thin-layer chromatogram of terpenoid hydrocarbon products made by TEAS and mutant TEAS enzymes using FPP as a substrate.

Brief Description of Tables

20 Table 1. X-ray crystallographic structural coordinates for 19 α -carbons found in the active site of a terpene synthase.

 Table 2. Interatomic distances in Angstroms between each α -carbon of Table 1. Each α -carbon occupies a sphere having a radius of 2.3 Angstroms. Interatomic distances are calculated from the center point of each sphere.

25 Table 3. X-ray crystallographic structural coordinates for 16 α -carbons found in the active site of a terpene synthase.

 Table 4. Interatomic distances in Angstroms between each α -carbon of Table 3. Each α -carbon occupies a sphere having a radius of 2.3 Angstroms. Interatomic distances are calculated from the center point of each sphere.

30 Table 5. X-ray crystallographic structural coordinates for nine α -carbons found in the active site of a terpene synthase.

 Table 6. Interatomic distances in Angstroms between each α -carbon of Table 5. Each α -carbon occupies a sphere having a radius of 2.3 Angstroms. Interatomic distances are calculated from the center point of each sphere.

35 Table 7. Ordered arrangement of R-groups not found associated with the α -carbons of Table 1.

Table 8. Ordered arrangement of R-groups not found associated with the α -carbons of Table 3.

Table 9. Ordered arrangement of R-groups not found associated with the α -carbons of Table 5.

5 Table 10. X-ray structural coordinates for TEAS having the substrate analog FHP bound in the active site.

Table 11. X-ray structural coordinates for TEAS in the absence of substrate.

10 Table 12. Alignment of residues 265-535 of TEAS with a limonene synthase, SEQ ID NO: 22, using the BLASTp alignment program.

Table 13. Alignment of residues 579 to 847 of SEQ ID NO:44 with SEQ ID NO:26, using the BLASTp program.

Table 14. Alignment of residues 265 to 535 of TEAS with SEQ ID NO:48, using the BLASTp program.

15 Table 15. Alignment of residues 307 to 593 of SEQ ID NO:50 with SEQ ID NO:56 using the BLASTp program.

Brief Description of the Sequence Listing

20 SEQ ID NO:1 is the DNA coding sequence for a tobacco 5-epi-aristolochene synthase (TEAS) protein. Genbank No: Q40577.

SEQ ID NO:2 is the amino acid sequence for the protein encoded by the DNA of SEQ ID NO:1.

SEQ ID NO:3 is the DNA coding sequence for a TEAS protein in which the codon for Trp273 has been changed to a codon for Glu.

25 SEQ ID NO:4 is the amino acid sequence for the W273E protein encoded by the TEAS DNA of SEQ ID NO:3.

SEQ ID NO:5 is the DNA coding sequence for a TEAS protein in which the codon for Tyr520 has been changed to a codon for Phe.

30 SEQ ID NO:6 is the amino acid sequence for the Y520F protein encoded by the TEAS DNA of SEQ ID NO:5.

SEQ ID NO:7 is the DNA coding sequence for a TEAS protein in which the codon for Tyr527 has been changed to a codon for Phe.

SEQ ID NO:8 is the amino acid sequence for the Y527F protein encoded by the TEAS DNA of SEQ ID NO:7.

35 SEQ ID NO:9 is the DNA coding sequence for a TEAS protein in which the codon for Trp273 has been changed to a codon for Ser and the codon for Cys440 has been changed to a codon for Trp.

SEQ ID NO:10 is the amino acid sequence for the W273S/C440W protein encoded by the TEAS DNA of SEQ ID NO:9.

SEQ ID NO:11 is the DNA coding sequence for TEAS proteins in which the codons for Tyr406 and Leu407 have each been changed to the nucleotides
5 NNS.

SEQ ID NO:12 is the amino acid sequence for the population of Y406X/L407X proteins encoded by the TEAS DNA of SEQ ID NO:11, where X is any naturally occurring amino acid.

10 SEQ ID NO:13 is a DNA primer sequence.

SEQ ID NO:14 is a DNA primer sequence.

SEQ ID NO:15 is a DNA primer sequence.

SEQ ID NO:16 is a DNA primer sequence.

SEQ ID NO:17 is a DNA primer sequence.

SEQ ID NO:18 is a DNA primer sequence.

15 SEQ ID NO:19 is the DNA coding sequence for a grand fir pinene synthase. Genbank Accession No: U87909.

SEQ ID NO:20 is the amino acid sequence for the protein encoded by the DNA of SEQ ID NO:19.

20 SEQ ID NO:21 is the DNA coding sequence for a spearmint limonene synthase. Genbank Accession No: L13459.

SEQ ID NO:22 is the amino acid sequence for the protein encoded by the DNA of SEQ ID NO:21.

25 SEQ ID NO:23 is the DNA coding sequence for a sage 1, 8 cineole synthase. Genbank Accession No: AF051899.

SEQ ID NO:24 is the amino acid sequence for the protein encoded by the DNA of SEQ ID NO:23.

SEQ ID NO:25 is the DNA coding sequence for a sage bornyl diphosphate synthase. Genbank Accession No: AF051900.

30 SEQ ID NO:26 is the amino acid sequence for the protein encoded by the DNA of SEQ ID NO:25.

SEQ ID NO:27 is the DNA coding sequence for a mint E-b-farnesene synthase. Genbank Accession No: AF024615.

SEQ ID NO:28 is the amino acid sequence for the protein encoded by the DNA of SEQ ID NO:27.

35 SEQ ID NO:29 is the DNA coding sequence for a grand fir myrcene synthase. Genbank Accession No: U87908.

SEQ ID NO:30 is the amino acid sequence for the protein encoded by the DNA of SEQ ID NO:29.

SEQ ID NO:31 is the DNA coding sequence for a potato vetaspiradiene synthase. Genbank Accession No: AB022598.

5 SEQ ID NO:32 is the amino acid sequence for the protein encoded by the DNA of SEQ ID NO:31.

SEQ ID NO:33 is the genomic DNA coding sequence for a cotton delta-cadinene synthase. Genbank Accession No: Y18484.

10 SEQ ID NOS:34-40 are the amino acid sequences for the exons encoded by the DNA of SEQ ID NO:33.

SEQ ID NO:41 is the DNA coding sequence for a castor bean casbene synthase. Genbank Accession No: L32134.

SEQ ID NO:42 is the amino acid sequence for the protein encoded by the DNA of SEQ ID NO:41.

15 SEQ ID NO:43 is the DNA coding sequence for a yew taxadiene synthase. Genbank Accession No: U48796.

SEQ ID NO:44 is the amino acid sequence for the protein encoded by the DNA of SEQ ID NO:43.

20 SEQ ID NO:45 is the DNA coding sequence for a grand fir E-alpha-bisabolene synthase. Genbank Accession No: AF006194.

SEQ ID NO:46 is the amino acid sequence for the protein encoded by the DNA of SEQ ID NO:45.

SEQ ID NO:47 is the DNA coding sequence for a grand fir delta-selinene synthase. Genbank Accession No: U92266.

25 SEQ ID NO:48 is the amino acid sequence for the protein encoded by the DNA of SEQ ID NO:47.

SEQ ID NO:49 is the DNA coding sequence for a grand fir gamma-humulene synthase. Genbank Accession No: U92267.

30 SEQ ID NO:50 is the amino acid sequence for the protein encoded by the DNA of SEQ ID NO:49.

SEQ ID NO:51 is the DNA coding sequence for a tomato germacrene C synthase. Genbank Accession No: AF035631.

SEQ ID NO:52 is the amino acid sequence for the protein encoded by the DNA of SEQ ID NO:51.

35 SEQ ID NO:53 is the DNA coding sequence for a sage +sabinene synthase. Genbank Accession No: AF051901.

SEQ ID NO:54 is the amino acid sequence for the protein encoded by the DNA of SEQ ID NO:53.

SEQ ID NO:55 is the DNA coding sequence for a grand fir abietadiene synthase. Genbank Accession No: U50768.

5 SEQ ID NO:56 is the amino acid sequence for the protein encoded by the DNA of SEQ ID NO:55.

SEQ ID NO:57 is the DNA coding sequence for a grand fir limonene synthase. Genbank Accession No: AF006193.

10 SEQ ID NO:58 is the amino acid sequence for the protein encoded by the DNA of SEQ ID NO:57.

Detailed Description

The following terms are used herein:

15 "α-carbon" refers to the chiral carbon atom found in an amino acid residue. Four substituents are covalently bound to the α-carbon, including an amino group, a carboxyl group, a hydrogen atom, and an R-group.

"R-group" refers to a substituent attached to the α-carbon of an amino acid residue that is not involved in peptide bond formation in a protein. An R-group is an important determinant of the overall chemical character of an amino acid. The
20 twenty naturally occurring amino acids found in proteins and the R-groups associated with the α-carbon of each amino acid are listed in Figure 2. The three-letter and one-letter abbreviations for naturally occurring amino acids are sometimes used herein to refer to the R-group associated with a particular amino acid.

"Naturally occurring amino acid" includes L-isomers of the twenty
25 amino acids naturally occurring in proteins. Naturally occurring amino acids are glycine, alanine, valine, leucine, isoleucine, serine, methionine, threonine, phenylalanine, tyrosine, tryptophan, cysteine, proline, histidine, aspartic acid, asparagine, glutamic acid, glutamine, arginine, and lysine. Unless specially indicated, all amino acids referred to in this application are in the L-form. Three-letter
30 and one-letter abbreviations are sometimes used herein to refer to naturally occurring amino acids. These abbreviations are known in the art.

"Unnatural amino acid" includes amino acids that are not naturally found in proteins. Examples of unnatural amino acids included herein are racemic mixtures of selenocysteine and selenomethionine. In addition, unnatural amino acids
35 include the D or L forms of norleucine, para-nitrophenylalanine, homophenylalanine,

para-fluorophenylalanine, 3-amino-2-benzylpropionic acid, homoarginine, D-phenylalanine, and the like.

5 "Positively charged amino acid" includes any naturally occurring or unnatural amino acid having an R-group that carries a positive charge under normal physiological conditions. Examples of positively charged, naturally occurring amino acids include arginine and lysine.

"Negatively charged amino acid" includes any naturally occurring or unnatural amino acid having an R-group that carries a negative charge under normal physiological conditions. Examples of negatively charged, naturally occurring amino acids include aspartic acid and glutamic acid.

"Hydrophobic amino acid" includes any naturally occurring or unnatural amino acid having an uncharged, nonpolar side chain under normal physiological conditions. Examples of naturally occurring hydrophobic amino acids are leucine, isoleucine, valine and methionine.

15 "Hydrophilic amino acid" includes any naturally occurring or unnatural amino acid having a charged polar side chain. Examples of naturally occurring hydrophilic amino acids include serine, threonine and cysteine.

"Mutant terpene synthase" or "mutated terpene synthase" refers to a synthase polypeptide having a primary amino acid sequence. The center point of the α -carbon of nine residues of the polypeptide is positioned within a sphere having a radius of 2.3 Angstroms; the center points of the nine spheres have the structural coordinates of Table 5 or coordinates which can be rotated and/or translated to coincide with the coordinates of Table 5. The relative interatomic distances between the nine α -carbons is ± 2.3 angstroms of the interatomic distances given in Table 6. Each α -carbon has an associated R-group. A mutant synthase differs from a non-mutant synthase in the ordered arrangement of R-groups associated with the nine α -carbons. A mutant synthase has an ordered arrangement of R-groups on the nine α -carbons other than the ordered arrangements of R-groups listed in Table 9. R-groups associated with other α -carbons of the synthase primary amino acid sequence may or may not be the same as in a non-mutated synthase.

30 In some embodiments, a mutant synthase refers to a synthase in which the center point of the α -carbon of sixteen residues of the polypeptide is positioned within a sphere having a radius of 2.3 Angstroms; the center points of the sixteen spheres have the structural coordinates of Table 3 or coordinates which can be rotated and/or translated to coincide with the coordinates of Table 3. The relative interatomic distances between the nine α -carbons is ± 2.3 angstroms of the interatomic distances given in Table 4. Each α -carbon has an associated R-group.

A mutant synthase differs from a non-mutant synthase in the ordered arrangement of R-groups associated with the sixteen α -carbons. A mutant synthase has an ordered arrangement of R-groups on the sixteen α -carbons other than the ordered arrangements of R-groups listed in Table 8. R-groups associated with other α -carbons of the synthase primary amino acid sequence may or may not be the same as in a non-mutated synthase.

In some embodiments, a mutant synthase refers to a synthase in which the center point of the α -carbon of nineteen residues of the polypeptide is positioned within a sphere having a radius of 2.3 Angstroms; the center points of the nineteen spheres have the three dimensional coordinates of Table 1 or coordinates which can be rotated and/or translated to coincide with the coordinates of Table 1. The relative interatomic distances between the nineteen α -carbons is ± 2.3 angstroms of the interatomic distances given in Table 2. Each α -carbon has an associated R-group. A mutant synthase differs from a non-mutant synthase in the ordered arrangement of R-groups associated with the nineteen α -carbons. A mutant synthase has an ordered arrangement of R-groups on the nineteen α -carbons other than the ordered arrangements of R-groups listed in Table 7. R-groups associated with other α -carbons of the synthase primary amino acid sequence may or may not be the same as in a non-mutated synthase.

"Nonmutated synthase" or "non-mutant synthase" includes a synthase having a primary amino acid sequence comprising nine, sixteen, or nineteen amino acid residues. The center point of each α -carbon of these residues is positioned within a sphere having a radius of 2.3 Angstroms; the center points of the spheres have the three dimensional coordinates of Tables 5, 3, or 1, respectively, or coordinates which can be rotated and/or translated to coincide with the coordinates of Tables 5, 3, or 1. The relative interatomic distances between the nine, sixteen, or nineteen α -carbons is ± 2.3 angstroms of the interatomic distances given in Tables 6, 4, or 2, respectively. Each α -carbon has an associated R-group. A non-mutant synthase has an ordered arrangement of R-groups on the nine, sixteen, or nineteen α -carbons as listed in Tables 9, 8, or 7, respectively.

"Degenerate variations thereof" refers to variants of a gene coding sequence by which the same polypeptide is encoded by different nucleotide sequences, due to the degeneracy of the genetic code. For example, synthases of the present invention have a primary amino acid sequence. Degenerate synthase variations are different nucleic acid coding sequences that nevertheless encode the same primary amino acid sequence due to the degeneracy of the genetic code.

"Expression" refers to transcription of a gene or nucleic acid molecule and the translation of that nucleic acid into a polypeptide. Expression of genes also involves processing of RNA into mRNA in eukaryotic systems. It is not necessary for the genes to integrate into the genome of a cell in order to achieve expression. This definition is not limited to expression in a particular system or a particular cell type and includes, without limitation, stable, transient, in vitro, and in vivo expression.

"Promoter" and "promoter regulatory element", refers to a nucleic acid that is involved in controlling expression of a gene. Promoter regulatory elements, and the like, from a variety of sources can be used efficiently to promote gene expression. Promoter regulatory elements include constitutive, tissue-specific, developmental-specific, inducible, subgenomic promoters, and the like. Promoter regulatory elements may also include certain enhancer elements or silencing elements that improve or regulate transcriptional efficiency.

"Active Site" refers to a site in a terpene synthase that binds the hydrophobic portion of a terpene substrate, GPP, FPP, and/or GGPP. The active site can, under certain conditions, catalyze a biosynthetic reaction that allows one or more reaction products to be produced.

"Altered enzymatic specificity" includes an alteration in the ability of a mutant synthase to use a particular terpene substrate or a change in the profile of reaction product(s) from a mutant synthase, compared to the substrate specificity of and the reaction products made by a corresponding non-mutated synthase. Altered specificity may include the ability of a synthase to exhibit different enzymatic parameters relative to a non-mutated synthase (K_m , V_{max} , etc), and/or to produce products that are different from those that are produced by a corresponding non-mutant synthase.

"Structure coordinates" or "structural coordinates" refers to Cartesian coordinates (x, y, and z positions) derived from mathematical equations involving Fourier synthesis as determined from patterns obtained via diffraction of a monochromatic beam of X-rays by the atoms (scattering centers) of a synthase molecule in crystal form. Diffraction data are used to calculate electron density maps of repeating protein units in the crystal (unit cell). Electron density maps are used to establish the positions of individual atoms within a crystal's unit cell. The absolute values for structural coordinates listed herein convey relative spatial relationships between atoms because the absolute values ascribed to structural coordinates can be changed by rotational and/or translational movement along the x, y and/or z axes, together or separately, while maintaining the same relative spatial relationships among atoms. Thus, a terpene synthase whose absolute values for a set of

structural coordinates can be rotationally or translationally adjusted to coincide with the particular values listed in Tables 1, 3, or 5 is considered to have the same structural coordinates as those of Tables 1, 3 or 5. An example of structural coordinates that coincide with the absolute values listed herein after rotation and/or translation are the coordinates of Table 11.

"Heavy atom derivatization" refers to a method of producing a chemically modified form of a synthase crystal. In practice, a crystal is soaked in a solution containing heavy atom salts or organometallic compounds, e. g., lead chloride, gold thiomalate, thimerosal, uranyl acetate and the like, which can diffuse through the crystal and bind to the protein's surface. Locations of the bound heavy atoms can be determined by X-ray diffraction analysis of the soaked crystal. The information is then used to construct phase information which can then be used to construct three-dimensional structures of the enzyme as described in Blundel, T. L., and Johnson, N. L., Protein Crystallography, Academic Press (1976).

"Unit cell" refers to a basic parallelepiped shaped block. Regular assembly of such blocks may construct the entire volume of a crystal. Each unit cell comprises a complete representation of the unit pattern, the repetition of which builds up the crystal.

"Mutagenesis" refers to the substitution of a different amino acid residue at a particular position in the primary amino acid sequence of a protein, thereby changing the R-group present at that position. Mutagenesis can be most easily performed by changing the coding sequence of a nucleic acid encoding the protein so that the coding sequence in the nucleic acid specifies an amino acid residue different from the residue initially present at that position.

"Space Group" refers to the arrangement of symmetry elements within a crystal.

"Molecular replacement" refers to the generation of a preliminary model of a synthase whose structural coordinates are unknown, by orienting and positioning a molecule whose structural coordinates are known within the unit cell of the unknown crystal so as best to account for the observed diffraction pattern of the unknown crystal. Phases can then be calculated from this model and combined with the observed amplitudes to give an approximate Fourier synthesis of the structure whose coordinates are unknown. This in turn can be subject to any of the several forms of refinement to provide a final, accurate structure of the unknown crystal (Lattman, E., 1985, in Methods in Enzymology, 115:55-77; Rossmann, MG., ed., "The Molecular Replacement Method" 1972, Int. Sci. Rev. Ser., No. 13, Gordon & Breach, New York). Using structure coordinates and interatomic distance matrices,

molecular replacement may be used to determine the structural coordinates of a crystalline mutant, homologue, or a different crystal form of terpene synthase.

"Recombinant protein" includes a protein that is chemically synthesized or derived biosynthetically from an isolated gene.

5 "Gene" includes naturally derived or genetically manipulated nucleic acids that contain the information needed to produce a polypeptide.

"Nucleic acid" includes any genetic material comprised of the nucleotides guanine, adenine, thymine, cytosine, uracil, inosine and the like. Nucleic acids may be single-, double-, or triple stranded. Nucleic acids may be
10 deoxyribonucleic acid or ribonucleic acid.

"Genetically manipulated" includes genes that have been modified to contain a different nucleotide sequence from that present in a preselected nucleic acid. Genes can be manipulated by synthetically or via traditional cloning, PCR, chemical gene synthesis, direct or random mutagenesis, and gene shuffling.
15 Genetically manipulated also includes the process of making genes that are degenerate variations of nucleic acids encoding preselected proteins.

"First domain" includes polypeptides having a first and second end wherein the first end can have an amino terminal amino acid with a free amino group and can be linked by a peptide bond to a second amino acid. The first end may also
20 be modified through acetylation and the like. The second end of the first domain may or may not have a free carboxyl terminal group.

"Second domain" includes polypeptides having a first and second end wherein the first end can have an amino terminal amino acid and can be linked by a peptide bond to a second amino acid. The second end of the second domain may or
25 may not have a carboxyl terminal group. Typically, the first end of the second domain is linked to the second end of the first domain via a peptide bond.

"Isoprenoid substrate" refers to the C₁₀, C₁₅, and C₂₀ molecules, named geranyl diphosphate (GPP), farnesyl diphosphate (FPP), and geranylgeranyl diphosphate (GGPP), respectively.

30 "Sequence identity" or "percent sequence identity" refers to the percentage of amino acids or nucleotides that occupy the same relative position when two protein sequences or nucleic acid sequences, a query sequence and a subject sequence, are aligned. The number of amino acid or nucleotide residues that are identical between both the subject and query sequences are counted, divided by
35 the number of residues in the query sequence, and multiplied by 100. The process is repeated until the alignment resulting in the highest percent sequence identity is found. Percent sequence identity can be determined by visual inspection and/or by

using various computer programs, e.g., MegAlign (DNASTAR, Inc., Madison, Wisconsin) or BLAST programs available on the world wide web from the National Center for Biotechnology Information (NCBI). Gaps of one or more residues may sometimes be inserted to maximize sequence alignments to structurally conserved domains of the query sequence, i.e., α -helices, β -sheets and loops.

5 "Monoterpene product" refers to linear, cyclized, and/or hydroxylated reaction products made from the substrate GPP. "Sesquiterpene product" refers to linear, cyclized, and/or hydroxylated reaction products made from the substrate FPP. "Diterpene product" refers to linear, cyclized, and/or hydroxylated reaction products
10 made from the substrate GGPP.

The present invention relates to terpene synthases and mutants thereof from which the position of specific α -carbon atoms and R-groups associated therewith comprising the active site can be determined in three-dimensional space. The invention also relates to structural coordinates of the synthases, use of the
15 structural coordinates to develop structural information related to synthase homologues, mutants, and the like, and to crystal forms of such synthases. Furthermore, the invention provides a method whereby α -carbon structural coordinates for atoms comprising the active site of a preselected terpene synthase can be used to develop synthases in which R-groups associated with active site α -
20 carbon atoms are different from the R-groups found in the preselected terpene synthase. In addition, the present invention provides for the production of novel terpene synthases based on the structural information provided herein and for the use of such synthases to make a variety of isoprenoid compounds.

The present invention further provides, for the first time, crystals of a
25 synthase, as exemplified by tobacco 5-epi-aristolochene synthase (TEAS), which are grown in the presence or absence of substrate and substrate analogues, thus allowing definition of the structural coordinates associated therewith. The structural coordinates allow determination of the α -carbon atoms comprising the active site and R-groups associated therewith. The crystals of the present invention belong to the
30 tetragonal space group $P4_12_12$; the unit cell dimensions vary by a few angstroms between crystals but on average $a = 126$ angstroms, $c = 122$ angstroms, $a=b$, $\alpha = 90^\circ$, $\beta = 90^\circ$, and $\gamma = 90^\circ$.

Structural coordinates are preferably obtained at a resolution of about 2.2 to about 2.8 angstroms for a synthase in the presence and in the absence of
35 bound substrate or substrate analog. Coordinates for a synthase with a substrate analog bound in the active site are given in Table 10. Coordinates for a synthase in

the absence of a substrate analog bound in the active site are given in Table 11. Those skilled in the art understand that a set of structure coordinates determined by X-ray crystallography is not without standard error. Therefore, for the purpose of this invention, any set of structure coordinates wherein the active site α -carbons of a
5 synthase, synthase homologue, or mutants thereof, have a root mean square deviation less than ± 2.3 angstroms when superimposed using the structural coordinates listed in Table 1, 3, or 5, are considered identical.

A schematic representation of the three-dimensional shape of a synthase is shown in Figure 1 which was prepared by RIBBONS (Carson and Bugg, 10 1986, J. Mol. Graphics, 4:121). The synthase shown in Figure 1 consists entirely of α -helices and short connecting loops and turns, organized into first and second structural domains.

In one embodiment, an isolated synthase of the invention comprises sixteen active site α -carbons having the structural coordinates of Table 3 and the
15 relative distances ± 2.3 angstroms of the distances given in Table 4. The active site α -carbons of Table 3 generally are not all contiguous, i.e., are not adjacent to one another in the primary amino acid sequence of a synthase, due to intervening amino acid residues between various active site α -carbons. On the other hand, it should be appreciated that some of the active site α -carbons can be adjacent to one another in
20 some instances. In the embodiment depicted in the TEAS Y527F protein (SEQ ID NO:8), for example, active site α -carbons are adjacent to one another in the primary amino acid sequence at positions 402, 403 and 404, respectively, whereas active site α -carbons at residues 273 and 294 are separated and thus are not adjacent. Thus, the numbering of active site α -carbons given in Tables 1, 2, 3, 4, 5, or 6 is merely for
25 convenience and such α -carbons may reside at any position in the primary amino acid sequence that achieves the structural coordinates given in Tables 1, 3, or 5 and the relative interatomic distances ± 2.3 angstroms given in Tables 2, 4, or 6.

An appropriate combination of R-groups, linked to active site α -carbons, can facilitate the formation of one or more desired reaction products. The
30 combination of R-groups selected for use in a terpene synthase of the invention can be any combination other than the ordered arrangements of R-groups and corresponding active site α -carbons shown in Tables 7, 8, or 9. An illustrative example of a suitable arrangement of R-groups and α -carbons is Cys, Trp, Ile, Ile, Ser, Thr, Thr, Tyr, Leu, Cys, Val, Thr, Phe, Asp, Tyr and Thr, associated with active
35 site α -carbons 1 to 16, respectively, of Table 3. Another example of a suitable arrangement of R-groups and α -carbons is Cys, Trp, Ile, Ile, Ser, Thr, Thr, Tyr, Leu,

Cys, Val, Thr, Tyr, Asp, Phe, and Thr at active site alpha-carbons 1 to 16, respectively, of Table 3. In some embodiments, a synthase of the invention may have primary amino acid sequences as listed in SEQ ID NO:4, SEQ ID NO:6, SEQ ID NO:8, and SEQ ID NO:10, DNA molecules encoding the same, which are listed in
5 SEQ ID NO:3, SEQ ID NO:5, SEQ ID NO:7, and SEQ ID NO:9, respectively, and degenerate variations thereof. Typically, R-groups found on active site α -carbons are those found in naturally occurring amino acids. See, e.g., Figure 2. In some embodiments, however, R-groups other than naturally occurring amino acids can be used.

10 Some arrangements of R-groups and active site α -carbons result in mutant terpene synthases that form reaction products. Such enzymatically active synthases and their corresponding genes are useful to make known terpenoid hydrocarbons, e.g., monoterpenes such as pinene, sesquiterpenes such as delta-cadinene and diterpenes such as abietadiene. Other enzymatically active synthases
15 can be used to make novel terpenoid products.

 Some arrangements of R-groups and active site α -carbons may result in mutant terpene synthases that do not form reaction product(s) at a desired rate. Such synthases and their genes are useful as controls in analyses of product formation by enzymatically active mutant synthases. Such synthases and their
20 genes can also be useful in analyses of translation of enzymatically active mutant synthase genes, or as nutritional supplements. Such synthases can be attached to Sepharose beads and used for affinity purification of isoprenoid compounds from crude preparations. In addition, such synthases and their genes can also be useful to develop reagents for various purposes, e.g., immunological reagents to monitor
25 expression of a terpene synthase protein or nucleic acid probes or primers to monitor inheritance of a terpene synthase gene in a plant breeding program.

 In some embodiments, the α -carbon backbone of a synthase first domain aligns structurally with the catalytic core of glycosyl hydrolases, as exemplified by glucoamylase (Brookhaven Protein Database (PDB) code 3GLY) from
30 *Aspergillus awamori* (Aleshin et al., 1994, J. Mol. Biol., 238:575) and endoglucanase CelD (PDB code ICLC) from *Clostridium thermocelum* (Juy et al., 1992, Nature, 357:89), and the α -carbon backbone of a synthase second domain, which contains the active site, aligns structurally with avian farnesyl diphosphate synthase (FPS), wherein the active site is comprised of 9, 16, or 19 amino acid residues with α -carbon
35 structural coordinates as listed in Tables 1, 3, or 5 and interatomic distances as

described in Tables 2, 4, or 6. Such α -carbons have an ordered arrangement of R-groups different from that observed in a non-mutated synthase.

In the present invention, the first domain forms a twisted α -barrel made up of eight short (10 to 15 amino acid residues) helices surrounding a surface cavity filled by ordered water molecules when hydrated. The second domain comprises a two-layered barrel of α -helices surrounding a hydrophobic and aromatic-rich active site pocket. Typically, the second domain contains a substrate binding site. As exemplified in Figure 1, helix H is disrupted between segments H1 and H2 by an amino acid such as proline, but its interhelical packing with helix G is accommodated by a corresponding kink in helix G between G1 and G2. Within this kink, hydrogen bonds between a hydroxyl group, such as that found on a threonine, and the carbonyl oxygen of other amino acids disrupt the main chain intrahelical hydrogen bonding of helix G thus assisting in producing the structure as determined.

As exemplified by TEAS, terpene synthases of the present invention can have a first domain segment comprising helices A, B, and C (an A-C loop), and a second domain comprising helices J and K (a J-K loop) (Figure 1). The ordering of these loops upon substrate binding results in a closed, solvent-inaccessible active site pocket. As the J-K loop becomes ordered, a lid-type structure is formed that clamps down over the active site entrance in the presence of substrate and an extended aromatic patch deep within the active site pocket is formed. As the A-C loop becomes ordered, it translates inward toward the active site, positioning certain R groups in this loop at or near the active site. Thus, substrate binding to the active site results in a change in protein conformation.

To identify or create mutant terpene synthases, sequence alignments can be performed to locate specific residues and α -carbons in a preselected polypeptide that have the structural coordinates and interatomic distances of Tables 1-2, 3-4 or 5-6. The preselected polypeptide is used as the subject sequence in the alignment, e.g., the full-length primary amino acid sequence, a region 190 residues in length, a region 220 residues in length, or a region 300 residues in length. The alignment can use residues 265 to 535 of TEAS (SEQ ID NO: 2), which includes the α -carbons of Tables 1, 3 or 5, as the query sequence to align with the preselected polypeptide. The preselected polypeptide and the query sequence can be aligned using the BLASTp 2.0.9 computer program with a BLOSUM 62 scoring matrix, an expect value of 10, a gap open value of 11, an x_dropoff value of 50, a gap extension value of 1, a wordsize of 3 and no filtering of low complexity sequences. As an alternative, the BLASTp 2.0.9 program can be used with a BLOSUM 50 scoring matrix, an expect value of 10, a gap open value 13, an x_dropoff value of 50, a gap

extension value of 2, a wordsize of 3 and no filtering of low complexity sequences. Other parameter values can also be used, e.g., a gap extension value from 0 to 4. See Altschul, et al., Nucl. Acids Res. 25:3389-3402.

Regions of the preselected polypeptide with significant sequence identity to residues 265-535 of TEAS, e.g., 20% or greater sequence identity, 25% or greater sequence identity, 35% or greater sequence identity, 40% or greater sequence identity, 50% or greater sequence identity, 60% or greater sequence identity, 70% or greater sequence identity, or 80% or greater sequence identity are examined for specific residues that align with the TEAS residues corresponding to those listed in Tables 1, 3, or 5. In some cases, the output of the computer program alignment identifies a specific residue in the preselected polypeptide for each of the nine, sixteen, or nineteen residues in the query sequence having the structural coordinates and interatomic distances of Tables 1-2, 3-4 or 5-6, with or without gaps introduced by the alignment program. In other cases, a gap is introduced by the alignment program in either the query sequence or the subject sequence such that no direct alignment or a misalignment occurs between one or more of the nine, sixteen, or nineteen residues in the query sequence that are of interest. In either case, the output can be visually inspected, and specific residues can be chosen in the subject sequence after adjusting the alignment so that alpha-helices and beta-sheet regions in the query sequence are maintained and that gaps or insertions in the subject sequence align with loop regions of the query sentence.

Sequence alignments suggest that other terpene synthases have regions with 20% or greater sequence identity to residues 265-535 of TEAS. Therefore, a region of a terpene synthase other than TEAS can be used as the query sequence, e.g., regions of terpene synthases given in SEQ ID NOS: 4, 6, 8, 10, 12, 20, 22, 24, 26, 28, 30, 32, 34-40, 42, 44, 46, 48, 50, 52, 54, 56, or 58, that have significant sequence identity to residues 265-535 of SEQ ID NO: 2. For example, large sequence insertions are present at the amino terminus in taxadiene synthase (SEQ ID NO: 44) with respect to TEAS, or are within solvent-exposed loops in the amino-terminal domain. Thus, regions of taxadiene synthase with greater than 20% sequence identity to SEQ ID NO: 2 are closer to the carboxy-terminal end, e.g., from residue 579 to residue 847 of SEQ ID NO: 44.

Useful regions of other terpene synthases that can be used as the query sequence include, without limitation, residues 343 to 606 of SEQ ID NO: 20, 316 to 586 of SEQ ID NO: 22, residues 352 to 622 of SEQ ID NO: 58, residues 272 to 540 encoded by SEQ ID NO: 33, residues 319 to 571 of SEQ ID NO: 42, residues 579 to 847 of SEQ ID NO: 44, residues 495 to 767 of SEQ ID NO: 46, residues 295

to 564 of SEQ ID NO: 48, residues 307 to 578 of SEQ ID NO: 50, residues 264 to 533 of SEQ ID NO: 52, residues 585 to 853 of SEQ ID NO: 56, residues 307 to 574 of SEQ ID NO: 54, residues 309 to 577 of SEQ ID NO: 24, residues 315 to 584 of SEQ ID NO: 26, residues 265 to 536 of SEQ ID NO: 28, residues 342 to 612 of SEQ ID NO: 30 and residues 273 to 541 of SEQ ID NO: 32.

One or more of the specific residues in the subject sequence that align with residues in the query sequence are mutated in the preselected polypeptide, e.g., by making mutations in a nucleic acid encoding the polypeptide. The mutant terpene synthase thus created can then be expressed in a host cell and the protein evaluated for enzymatic activity, if desired.

Mutant proteins of the present invention may be prepared in a number of ways including but not limited to oligonucleotide-directed mutagenesis, deletion, chemical mutagenesis, and the like. One or more R-groups associated with the active site α -carbon atoms in a terpene synthase are changed by altering the nucleotide sequence of the corresponding gene. For example, a mutation can be introduced into SEQ ID NO:1, the nucleotide sequence for TEAS, at codons encoding one or more of the following sixteen α -carbons: α -carbon 1 = Cys 270; α -carbon 2 = Trp 273; α -carbon 3 = Ile 294; α -carbon 4 = Ile 297; α -carbon 5 = Ser298; α -carbon 6 = Thr 402; α -carbon 7 = Thr 403; α -carbon 8 = Tyr 404; α -carbon 9 = Leu 407; α -carbon 10 = Cys 440; α -carbon 11 = Val 516; α -carbon 12 = Thr 519; α -carbon 13 = Tyr 520; α -carbon 14 = Asp 525; α -carbon 15 = Tyr 527; or α -carbon 16 = Thr 528. The protein encoded by the mutant gene is then produced by expressing the gene in, for example, a bacterial or plant expression system. Alternatively, synthase mutants may be generated by site specific replacement of a particular amino acid with an unnaturally occurring amino acid. As such, synthase mutants may be generated through replacement of an amino acid residue or a particular cysteine or methionine residue with selenocysteine or selenomethionine. This may be achieved by growing a host organism capable of expressing either the wild-type or mutant polypeptide on a growth medium depleted of natural cysteine or methionine or both and growing on medium enriched with either selenocysteine, selenomethionine, or both. These and similar techniques are described in Sambrook et al., (Molecular Cloning, A Laboratory Manual, 2nd Ed. (1989) Cold Spring Harbor Laboratory Press).

Another suitable method of creating mutant synthases of the present invention is based on a procedure described in Noel and Tsal (1989) J. Cell. Biochem., 40:309-320. In so doing, the nucleic acid encoding the synthase can be synthetically produced using oligonucleotides having overlapping regions, the oligonucleotides being degenerate at specific bases so that mutations are induced.

According to the present invention, nucleic acid sequences encoding a mutated synthase can be produced by the methods described herein, or any alternative methods available to the skilled artisan. In designing the nucleic acid sequence (gene) of interest, it may be desirable to reengineer the gene for improved expression in a particular expression system. For example, it has been shown that many bacterially derived genes do not express well in plant systems. In some cases, plant-derived genes do not express well in bacteria. This phenomenon may be due to the non-optimal G+C content or A+T content of the gene relative to the expression system being used. For example, the very low G+C content of many bacterial genes results in the generation of sequences mimicking or duplicating plant gene control sequences that are highly A+T rich. The presence of A+T rich sequences within the genes introduced into plants (e.g., TATA box regions normally found in gene promoters) may result in aberrant transcription of the gene(s). In addition, the presence of other regulatory sequences residing in the transcribed mRNA (e.g. polyadenylation signal sequences (AAUAAA) or sequences complementary to small nuclear RNAs involved in pre-mRNA splicing) may lead to RNA instability. Therefore, one goal in the design of genes is to generate nucleic acid sequences that have a G+C content that affords mRNA stability and translation accuracy for a particular expression system.

Due to the plasticity afforded by the redundancy of the genetic code (i.e., some amino acids are specified by more than one codon), evolution of the genomes of different organisms or classes of organisms has resulted in differential usage of redundant codons. This "codon bias" is reflected in the mean base composition of protein coding regions. For example, organisms with relatively low G+C contents utilize codons having A or T in the third position of redundant codons, whereas those having higher G+C contents utilize codons having G or C in the third position. Therefore, in reengineering genes for expression, one may wish to determine the codon bias of the organism in which the gene is to be expressed. Looking at the usage of the codons as determined for genes of a particular organism deposited in GenBank can provide this information. After determining the bias thereof, the new gene sequence can be analyzed for restriction enzyme sites as well as other sites that could affect transcription such as exon:intron junctions, polyA addition signals, or RNA polymerase termination signals.

Genes encoding synthases can be placed in an appropriate vector, depending on the artisan's interest, and can be expressed using a suitable expression system. An expression vector, as is well known in the art, typically includes elements that permit replication of said vector within the host cell and may

contain one or more phenotypic markers for selection of cells containing said gene. The expression vector will typically contain sequences that control expression such as promoter sequences, ribosome binding sites, and translational initiation and termination sequences. Expression vectors may also contain elements such as
5 subgenomic promoters, a repressor gene or various activator genes. The artisan may also choose to include nucleic acid sequences that result in secretion of the gene product, movement of said product to a particular organelle such as a plant plastid (see U.S. Patent Nos. 4,762,785; 5,451,513 and 5,545,817), or other sequences that increase the ease of peptide purification, such as an affinity tag.

10 A wide variety of expression control sequences are useful in expressing mutated synthases when operably linked thereto. Such expression control sequences include, for example, the early and late promoters of SV40 for animal cells, the lac system, the trp system, major operator and promoter systems of phage λ , and the control regions of coat proteins, particularly those from RNA viruses
15 in plants. In *E. coli*, a useful transcriptional control sequence is the T7 RNA polymerase binding promoter, which can be incorporated into a pET vector as described by Studier et al., (1990) *Methods Enzymology*, 185:60-89.

For expression, a desired gene should be operably linked to the expression control sequence and maintain the appropriate reading frame to permit
20 production of the desired synthase. Any of a wide variety of well-known expression vectors are of use in the present invention. These include, for example, vectors consisting of segments of chromosomal, non-chromosomal and synthetic DNA sequences such as those derived from SV40, bacterial plasmids (including those from *E. coli* such as col E1, pCR1, pBR322 and derivatives thereof, pMB9), wider
25 host range plasmids such as RP4, phage DNA such as phage λ , NM989, M13, and other such systems as described by Sambrook et al., (*Molecular Cloning, A Laboratory Manual*, 2nd Ed. (1989) Cold Spring Harbor Laboratory Press).

A wide variety of host cells are available for expressing synthase mutants of the present invention. Such host cells include, without limitation, bacteria
30 such as *E. coli*, *Bacillus* and *Streptomyces*, fungi, yeast, animal cells, plant cells, insect cells, and the like. Preferred embodiments of the present invention include terpene synthase mutants that are expressed in *E. coli* or in plant cells. Said plant cells can either be in suspension culture or a culture on a solid support such as an agar-based medium.

35 Genes encoding synthases of the present invention can also be expressed in transgenic plant cells. In order to produce transgenic plants, vectors containing a nucleic acid construct encoding a mutant terpene synthase are inserted

into the plant genome. Preferably, these recombinant vectors are capable of stable integration into the plant genome. One variable in making a transgenic plant is the choice of a selectable marker gene. A selectable marker gene is used to identify transformed cells against a high background of untransformed cells. Such selectable
5 marker genes include but are not limited to aminoglycoside phosphotransferase gene of transposon Tn5 (Aph II) which encodes resistance to the antibiotics kanamycin, neomycin, and G418, as well as those genes which encode for resistance or tolerance to glyphosate, hygromycin, methotrexate, phosphinothricin, imidazolinones, sulfonylureas, and triazolopyrimidine herbicides, such as chlorosulfuron,
10 bromoxynil, dalapon and the like. In addition to a selectable marker gene, it may be desirable to use a reporter gene. In some instances a reporter gene may be used with a selectable marker. Reporter genes allow the detection of transformed cell and may be used at the discretion of the artisan. A list of these reporter genes is provided in K. Weising et al., 1988, Ann. Rev. Genetics, 22:421.

15 The genes are expressed either by promoters expressing in all tissues at all times (constitutive promoters), by promoters expressing in specific tissues (tissue-specific promoters), promoters expressing at specific stages of development (developmental promoters), and/or promoter expression in response to a stimulus or stimuli (inducible promoters). The choice of these is at the discretion of the artisan.

20 Several techniques exist for introducing foreign genes into plant cells, and for obtaining plants that stably maintain and express the introduced gene. Such techniques include acceleration of genetic material coated directly into cells (U.S. Patent 4,945,050). Plant may also be transformed using Agrobacterium technology (U.S. Patents 5,177,010, 5,104,310, 5,149,645, 5,469,976, 5,464,763, 4,940,838,
25 4,693,976, 5,591,616, 5,231,019, 5,463,174, 4,762,785, 5,004,863, and 5,159,135; European Patent Applications 116718, 290799, 320500, 604662, 627752, 0267159, and 0292435. Other transformation technologies include whiskers technology, see U. S. Patents 5,302,523 and 5,464,765. Electroporation technology has also been used to transform plants, see WO 87/06614, WO 92/09696 and WO 93/21335 and
30 U.S. Patents 5,472,869 and 5,384,253. Viral vector expression systems can also be used such as those described in U.S. Patent 5,316,931, 5,589,367, 5,811,653, and 5,866,785.

In addition to numerous technologies for transforming plants, the type of tissue that is contacted with the genes of interest may vary as well. Suitable tissue
35 includes, but is not limited to, embryogenic tissue, callus tissue, hypocotyl, meristem and the like. Almost all plant tissues may be transformed during dedifferentiation using the appropriate techniques described herein.

Regardless of the transformation system used, a gene encoding a mutant synthase is preferably incorporated into a gene transfer vector adapted to express said gene in a plant cell by including in the vector an expression control sequence (plant promoter regulatory element). In addition to plant promoter
5 regulatory elements, promoter regulatory elements from a variety of sources can be used efficiently in plant cells to express foreign genes. For example, promoter regulatory elements of bacterial origin, such as the octopine synthase promoter, the nopaline synthase promoter, the mannopine synthase promoter may be used. Promoters of viral origin, such as the cauliflower mosaic virus (35S and 19S) are also
10 desirable. Plant promoter regulatory elements also include, but are not limited to, ribulose-1,6-bisphosphate carboxylase small subunit promoter, beta-conglycinin promoter, phaseolin promoter, ADH promoter, heat-shock promoters, and tissue specific promoters and the like. Numerous promoters are available to skilled artisans for use at their discretion.

15 It should be understood that not all expression vectors and expression systems function in the same way to express the mutated gene sequences of the present invention. Neither do all host cells function equally well with the same expression system. However, one skilled in the art may make a selection among these vectors, expression control sequences, and host without undue
20 experimentation and without departing from the scope of this invention.

Once a synthase of the present invention is expressed, the protein obtained therefrom can be purified so that structural analysis, modeling, and/or biochemical analysis can be performed, as exemplified herein. The nature of the protein obtained can be dependent on the expression system used. For example,
25 genes, when expressed in mammalian or other eukaryotic cells, may contain latent signal sequences that may result in glycosylation, phosphorylation, or other post-translational modifications, which may or may not alter function. Once the proteins are expressed, they can be easily isolated and purified using techniques common to the person having ordinary skill in the art of protein biochemistry and as described in
30 Colligan et al., (1997) Current Protocols in Protein Science, Chanda, V.B., Ed., John Wiley & Sons, Inc. Such techniques often include the use of cation-exchange or anion-exchange chromatography, gel filtration-size exclusion chromatography, and the like. Another technique that may be commonly used is affinity chromatography. Affinity chromatography can include the use of antibodies, substrate analogs, or
35 histidine residues (His-tag technology).

Once purified, mutants of the present invention may be characterized by any of several different properties. For example, such mutants may have altered

active site surface charges of one or more charge units. In addition, the mutants may have an altered substrate specificity or spectrum of reaction product relative to a non-mutated synthase.

The present invention allows for the characterization of mutant
5 terpene synthase by crystallization followed by X-ray diffraction. Polypeptide crystallization occurs in solutions where the polypeptide concentration exceeds its solubility maximum (i.e., the polypeptide solution is supersaturated). Such solutions may be restored to equilibrium by reducing the polypeptide concentration, preferably through precipitation of the polypeptide crystals. Often polypeptides may be induced
10 to crystallize from supersaturated solutions by adding agents that alter the polypeptide surface charges or perturb the interaction between the polypeptide and bulk water to promote associations that lead to crystallization.

Compounds known as "precipitants" are often used to decrease the solubility of the polypeptide in a concentrated solution by forming an energetically
15 unfavorable precipitating depleted layer around the polypeptide molecules (Weber, 1991, *Advances in Protein Chemistry*, 41:1-36). In addition to precipitants, other materials are sometimes added to the polypeptide crystallization solution. These include buffers to adjust the pH of the solution and salts to reduce the solubility of the polypeptide. Various precipitants are known in the art and include the following:
20 ethanol, 3-ethyl-2,4-pentanediol, and many of the polyglycols, such as polyethylene glycol.

Commonly used polypeptide crystallization methods include the following techniques: batch, hanging drop, seed initiation, and dialysis. In each of these methods, it is important to promote continued crystallization after nucleation by
25 maintaining a supersaturated solution. In the batch method, polypeptide is mixed with precipitants to achieve supersaturation, the vessel is sealed and set aside until crystals appear. In the dialysis method, polypeptide is retained in a sealed dialysis membrane that is placed into a solution containing precipitant. Equilibration across the membrane increases the polypeptide and precipitant concentrations thereby
30 causing the polypeptide to reach supersaturation levels.

In the preferred hanging drop technique (McPherson, 1976, *J. Biol. Chem.*, 6300-6306), an initial polypeptide mixture is created by adding a precipitant to a concentrated polypeptide solution. The concentrations of the polypeptide and precipitants are such that in this initial form, the polypeptide does not crystallize. A
35 small drop of this mixture is placed on a glass slide that is inverted and suspended over a reservoir of a second solution. The system is then sealed. Typically, the second solution contains a higher concentration of precipitant or other dehydrating

agent. The difference in the precipitant concentrations causes the protein solution to have a higher vapor pressure than the solution. Since the system containing the two solutions is sealed, an equilibrium is established, and water from the polypeptide mixture transfers to the second solution. This equilibrium increases the polypeptide and precipitant concentration in the polypeptide solution. At the critical concentration of polypeptide and precipitant, a crystal of the polypeptide may form.

Another method of crystallization introduces a nucleation site into a concentrated polypeptide solution. Generally, a concentrated polypeptide solution is prepared and a seed crystal of the polypeptide is introduced into this solution. If the concentration of the polypeptide and any precipitants are correct, the seed crystal will provide a nucleation site around which larger crystal forms. In preferred embodiments, the crystals of the present invention are formed in hanging drops with 15% PEG 8000; 200 mM magnesium acetate or magnesium chloride, 100 mM 3-(N-morpholino)-2-hydroxypropanesulfonic acid (pH 7.0), 1 mM dithiothreitol as precipitant.

Some proteins may be recalcitrant to crystallization. However, several techniques are available to the skilled artisan to induce crystallization. The removal of polypeptide segments at the amino or carboxyl terminal end of the protein may facilitate production of crystalline protein samples. Removal of such segments can be done using molecular biology techniques or treatment of the protein with proteases such as trypsin, chymotrypsin, subtilisin. Such procedures can result in the removal of flexible polypeptide segments that may negatively affect crystallization.

The crystals so produced have a wide range of uses. For example, high quality crystals are suitable for X-ray or neutron diffraction analysis to determine the three-dimensional structure of a mutant synthase and to design additional mutants thereof. In addition, crystallization can serve as a further purification method. In some instances, a polypeptide or protein will crystallize from a heterogeneous mixture into crystals. Isolation of such crystals by filtration, centrifugation, etc., followed by redissolving the polypeptide affords a purified solution suitable for use in growing the high-quality crystals needed for diffraction studies. The high-quality crystals may also be dissolved in water and then formulated to provide an aqueous solution having other uses as desired.

Because synthases may crystallize in more than one crystal form, the structural coordinates of α -carbons of an active site determined from a synthase or portions thereof, as provided by this invention, are particularly useful to solve the structure of other crystal forms of synthases. The structural coordinates, as provided

herein, may also be used to solve the structure of synthases having α -carbons position within the active sites in a manner similar to the wild-type yet having R-groups that may or may not be identical. Furthermore, the structural coordinates disclosed herein may be used to determine the structure of the crystalline form of other proteins with significant amino acid or structural homology to any functional domain of a synthase. One method that may be employed for such purpose is molecular replacement. In this method, the unknown crystal structure, whether it is another crystal form of a synthase, a synthase having a mutated active site, or the crystal of some other protein with significant sequence identity and/or structural homology of a synthase may be determined using the coordinates given in Tables 10 and/or 11. This method provides sufficient structural form for the unknown crystal more efficiently than attempting to determine such information ab initio. In addition, this method can be used to determine whether or not a given synthase in question falls within the scope of this invention.

As further disclosed herein, synthases and mutants thereof may be crystallized in the presence or absence of substrates and substrate analogs. The crystal structures of a series of complexes may then be solved by molecular replacement and compared to that of the wild-type to assist in determination of suitable replacements for R-groups within the active site, thus making synthase mutants according to the present invention.

All mutants of the present inventions may be modeled using the information disclosed herein without necessarily having to crystallize and solve the structure for each and every mutant. For example, one skilled in the art may use one of several specialized computer programs to assist in the process of designing synthases having mutated active sites. Examples of such programs can be as follows: GRID (Goodford, 1985, J. Med. Chem., 28:849-857); MCSS (Miranker and Karplus, 1991, Proteins: Structure, Function and Genetics, 11:29-34); AUTODOCK (Goodsell and Olsen, 1990, Proteins: Structure, Function, and Genetics, 8:195-202); and DOCK (Kuntz et al., 1982, J. Mol. Biol., 161:269-288). In addition, specific computer programs are also available to evaluate specific substrate-active site interactions and the deformation energies and electrostatic interactions resulting therefrom. MODELLER is a computer program often used for homology or comparative modeling of the three-dimensional structure of a protein. A. Sali & T.L. Blundell. J.Mol.Biol. 234, 779-815, 1993. A preselected polypeptide sequence to be modeled is aligned with one or more terpene synthases whose crystal structures are known and the MODELLER program is used to calculate a full-atom model, based on optimum satisfaction of spatial restraints. Such restraints can include, inter alia,

homologous structures, fluorescence spectroscopy, NMR experiments, or atom-atom potentials of mean force.

The present invention enables synthase mutants to be made and crystal structures thereof to be solved. Moreover, by virtue of the present invention, the location of the active site and the interface of substrate therewith permit the identification of desirable R-groups for mutagenesis. The particular embodiments of this invention are further exemplified in the Examples. However, those skilled in the art will readily appreciate that the specific experiments detailed are only illustrative of the invention as described more fully in the claims, which follow thereafter.

EXAMPLE 1

GENERATION OF MUTANT TEAS GENES

15 Construct generation and expression.

All mutant enzymes were constructed by the QuickChange method (Stratagene). Manufacturer's instructions were followed, except as noted. Mutations were confirmed by DNA sequencing, and plasmids containing the desired mutation were used to transform BL-21(DE3) expression cells. Protein was expressed, purified, and stored at -80°C.

TEAS W273S. The TEAS W273S mutant was generated from a TEAS-pET28b(+) template using the following primers:

GTTGAATGCTACTTTTCGGCATTAGGAGTTTAT (sense) (SEQ ID NO:13) and
ATAAACTCCTAATGCCGAAAAGTAGCATTCAAC (antisense) (SEQ ID NO:14).

25 Mutagenesis was carried out according to the manufacturer's instructions, except that sense and antisense strands were generated in separate reactions. For each, 30 plasmid-copying cycles of one minute, annealing at 55°C and 16 minutes extension at 68°C were carried out. The two reaction mixtures were then combined, heated to 95°C for 2.5 minutes, and cooled to room temperature before DpnI treatment.

30 **TEAS C440W.** The TEAS C440W mutant was generated from the TEAS-pET28b(+) template using the following primers:

GCTAGTGTAATTATATGGCGAGTTATCGATGAC
(sense) (SEQ ID NO:15) and GTCATCGATAACTCGCCATATAATTACACTAGC
(antisense) (SEQ ID NO:16).

35 **TEAS W273S/C440W.** The TEAS C440W/W273S mutant was constructed from a TEAS W273S-pET28b(+) template using the primers described for generation of TEAS C440W.

TEAS 406/407 random library. For generation of a library of TEAS mutants with random amino acids at positions 406 and 407, two 50 microliter QuickChange reactions were carried out with the TEAS-pET28b(+) template and the primers

5 GCACTAGCAACTACCACATATTACNNSNNSGCGACAACATCGTATTTGGGCATG (sense) (SEQ ID NO:17) and

CATGCCCAAATACGATGTTGTCGCSNNSNNGTAATATGTGGTAGTTGCTAGTGC (antisense) (SEQ ID NO:18), in which N denotes A, C, G, or T and S denotes C or G. By this choice of nucleotides, the reaction included primers which coded for all

10 possible amino acid combinations at positions 406 and 407. No adjustment was made for differing numbers of codons among amino acids. In order to ensure efficient reactions, and to minimize the preference for hybridization of wild-type primers to the template, the primers were designed to be longer than those used to generate the mutations described above. In addition, they were HPLC purified prior

15 to use. After 18 cycles of plasmid copying, the reaction was incubated for two hours with DpnI, ethanol precipitated, and redissolved in 5 microliters water. Each of four 40 microliter aliquots of *E. coli* NovaBlue (Novagen) cells were electroporated with 1.5 microliters of the redissolved DNA. After a recovery period, the cells were plated on kanamycin-LB-agar plates. In order to transfer the newly constructed plasmids to

20 expression cells, the colonies were scraped from all four plates, and used to start an 8 mL culture grown in liquid LB medium at 37°C for 8 hours. Plasmid purified from this culture was used to transform 20 microliters of competent BL-21(DE3) cells.

For storage of the constructs, each individual colony was used to inoculate 100 microliters of LB medium containing kanamycin (50 micrograms/mL) in

25 96-well culture plates. The cells were grown at 37°C until the A_{600} reached approximately one; 100 microliters of 30% glycerol in LB were then added, and the plates were frozen at -80°C. A set of randomly selected colonies were grown from individual glycerol stocks of some colonies, and plasmids were extracted for sequencing. Approximately 30 percent of the colonies were found to be wild-type.

30 Nucleotide and amino acid sequences for TEAS 406/407 mutant genes and proteins are shown in SEQ ID NOS:11 and 12.

TEAS Y520F The tyrosine residue at position 520 of SEQ ID No:2 was changed to a phenylalanine residue by site-directed mutagenesis with primers, in a manner similar to that described above. For Y520F the TAT codon was changed

35 to TTC. The nucleotide sequence of the mutant gene is shown in SEQ ID No:5.

TEAS Y527F The tyrosine residue at position 527 of SEQ ID No:2 was changed to a phenylalanine residue by site-directed mutagenesis with primers,

in a manner similar to that described above. For Y527F, the TAC codon at position 527 of the TEAS amino acid sequence was changed to TTC. The nucleotide sequence of the mutant TEAS Y527F gene is shown in SEQ ID No: 7.

TEAS W273E The tryptophan residue at position 273 of SEQ ID No:2
5 was changed to a phenylalanine residue by site-directed mutagenesis with primers, in a manner similar to that described above. For W273E, the TGG codon at position 273 of the TEAS amino acid sequence was changed to GAG. The nucleotide sequence of the mutant gene is shown in SEQ ID No.:3.

10

EXAMPLE 2

EXPRESSION AND ISOLATION OF SYNTHASE POLYPEPTIDES

Unless otherwise noted, mutated and non-mutated TEAS proteins
15 were expressed in *Escherichia coli*, purified by metal chelation, anion exchange, and gel filtration chromatography.

Constructs of TEAS and mutant TEAS proteins in the vector pET-28b(+) (Novagen) were expressed in *E. coli* cells. For a typical protein preparation of any of these enzymes, *E. coli* strain BL21(DE3) cells containing the plasmid
20 construct were grown at 37°C in 4 X 1L terrific broth to an $A_{600} = 1.0$. The temperature was dropped to 22°C, and protein expression was induced by adding IPTG to a final concentration of 0.1 mM. After 15-20 h, the cells were harvested by centrifugation, resuspended in 5mL buffer A (20 mM Tris, 500 mM NaCl, 20 mM imidazole, pH 7.9) per 1g cells (wet weight), and stirred for 0.5 h at 4°C. The cells
25 were then lysed by sonication, and the resulting lysate was centrifuged for 0.7 h at 82,000 xg. The supernatant, containing the protein, was loaded over a 2-3 mL Ni^{2+} chelating histidine affinity column (Qiagen) equilibrated in buffer A, and the column was washed with additional buffer A until the A_{280} of the eluent returned to baseline. The protein was then eluted with a 20-200 mM imidazole gradient in buffer A.
30 Protein-containing fractions were pooled and dialyzed against buffer B (50 mM HEPES, 5mM $MgCl_2$, 1mM DTT), then loaded onto an 8 mL MonoQ cation-exchange column (Pharmacia). The column was washed with 20 column volumes buffer B, and the protein was eluted with a 0-500 mM NaCl gradient in buffer B. The resulting protein was further purified by gel filtration on a Superdex-200 column (Pharmacia) in
35 50 mM Tris, 100 mM NaCl, 5mM $MgCl_2$, 1mM DTT, pH 8.0. Purified protein was then dialyzed against 5mM Tris, 5mM NaCl, 1mM DTT, pH 8.0, concentrated to 18-22 mg/mL, and stored at -80°C in 100° L aliquots until needed.

EXAMPLE 3
CRYSTALLIZATION AND STRUCTURAL ANALYSIS OF SYNTHASE
POLYPEPTIDES

5

Crystal Growth and Microseeding: All crystallization attempts were carried out by the hanging-drop vapor diffusion method. Concentrated protein was mixed with an equal volume (2-5 uL each) of reservoir solution on a plastic cover slip. The cover slip was then inverted over a well of a plastic 24-well tissue culture plate, containing 0.5-1.0 mL of reservoir solution, and sealed by a layer of vacuum grease between the well and cover slip. The plates were incubated at 4°C while the protein concentration in the hanging drop slowly increased by vapor diffusion. Approximately 300 different reservoir solutions, ranging pH 4.5-9 with a variety of precipitants and added salts, were assayed for crystallization of TEAS (SEQ ID NO:2). TEAS crystallized with a reservoir solution of 15% PEG 8000, 100 mM MOPSO (3-[N-morpholino]-2-hydroxypropanesulfonic acid), 200 mM magnesium acetate, 1 mM DTT, pH 6.9-7.3. For microseeding, an existing crystal was crushed in a few uL of precipitant solution, then diluted to 50 microliters. After initial centrifugation to remove large particles, the suspension was serially diluted with additional precipitant solution, and a small volume of a diluted seed stock was added to each new crystallization drop. For macroseeding, crystals which were no longer rapidly growing (usually 2 weeks after drops were set up), were "rinsed" by serially transferring them through two to three drops of reservoir solution. The crystal was then transferred to a fresh drop containing protein and reservoir solution, and equilibrated against a reservoir solution as in the initial growth. Individual crystals varied in their degree of internal order. In some cases, several crystals were screened to identify a well-diffracting crystal with low mosaicity.

Data collection: Prior to data collection, crystals were transferred to a drop of reservoir solution, or reservoir solution containing a compound to be soaked into the crystal. A small volume of cryoprotectant solution (15% PEG8000, 100 mM MOPSO, 200 mM Mg acetate, 20% ethylene glycol, 1mM DTT, pH 7) was then added to the drop. After a short equilibration time (1-5 minutes), the crystal was transferred to a drop of cryoprotectant, or cryoprotectant with soaking compound added. After another short equilibration time, the crystal was picked up on a nylon loop, and quickly mounted for data collection in a stream of cold nitrogen gas (90-110K).

The TEAS crystals belonged to the tetragonal space group $P4_12_12_1$; the unit cell dimensions varied by a few angstroms between crystals, but on average $a = 126 \text{ \AA}$, $c = 122 \text{ \AA}$. The uncomplexed TEAS structure was initially refined to 2.8 \AA (Table 11) against data collected from a crystal grown in the presence of 2 mM FHP (Table 10). Electron density at the active site allowed unambiguous modeling of FHP, the A-C and J-K loops, and nine additional residues at the NH_2 terminus. The refined TEAS-FHP model consisted of residues 17 to 548, three Mg^{2+} ions, 150 water molecules, and one FHP molecule. The three-dimensional coordinates for TEAS in the presence of bound substrate is shown in Table 10. The three-dimensional coordinates for TEAS in the absence of FHP is shown in Table 11.

Crystals of TEAS complexed with trifluoro-farnesyl diphosphate (F3-FPP) were also prepared. In these crystals, a well-ordered diphosphate binding pocket was also observed. The A-C loop and the NH_2 -terminal segment exhibited well-defined electron density, the A-C loop was translated toward the active site, and there was strong electron density for the diphosphate moiety of F3-FPP. The hydrophobic pocket, however, remained flexible; the J-K loop and the farnesyl moiety of F3-FPP were disordered.

Homology models were created and energy-minimized using the Swiss PDB viewer interface of the SwissModel program (Peitsch MC (1996), Biochem. Soc. Trans., 24:274-279 and Guex N. and Peitsch MC, 1997, Electrophoresis., 18:2714-2723). Active site volumes were calculated with VOIDOO (Kleywegt, G.J., and Jones, T.A., CCP4/ESF-EACBM Newsletter on Protein Crystallography., 29, 26-28, 1993). To make closed active site cavities, the energy-minimized diphosphate moiety from the modeled TEAS cyclase reaction was appended to the residue equivalent to TEAS D301.

TEAS W273S crystal structures. Two TEAS W273S structures, in the presence of FHP, were determined from different crystals; both crystals appeared to be well ordered, as clear main-chain and side-chain density were apparent for residues throughout the protein, including the frequently mobile helices D1, D2, and E. Initial difference electron density maps from both crystals immediately revealed the W273S mutations. The two crystals were designated W273S-1 and W273S-2.

In each structure, the loops surrounding the active site were ordered, resulting in a closed active site pocket. The A/C loop in each structure was translated toward the active site, forming part of its outer rim, as observed in the wild-type TEAS/FHP complex. However, while the J/K loop of W273S-1 adopted the same conformation observed in the wild-type TEAS/FHP complex, the same loop in W273S-2 adopted a different conformation. In this conformation of the J/K loop,

Tyr527 moved away from the side chain of residue 273. In addition, Tyr520 and Asp525 were placed distal to the side chain of Asp444. Hydrogen bonds previously observed between the J/K loop, Arg266, and the N-terminal loop were also missing in the W273S-2 structure.

5 The W273S-2 conformation does not appear to be an effect of the W273S mutation, as it was also observed in a wild-type TEAS crystal soaked with the epi-aristolochene mimic deoxycapsidiol, despite the fact that no electron density was readily apparent for the deoxycapsidiol molecule in that structure. Further, the TEAS active site loops were distant from crystal contacts, and their conformations were not
10 likely to be artifacts of crystal packing. It is possible that at different stages of the TEAS reaction, the enzyme's J/K loop exists in different, defined conformations, and that each of these crystal structures has captured an image of a different conformation. In both W273S structures, residues other than Arg266 and those on the J/K loop did not undergo significant rearrangement from the conformations
15 observed in wild-type TEAS.

 In each W273S crystal structure, electron density in the active site suggested that the substrate mimic FHP binds in multiple conformations. Some regions of this density possibly represented bound water molecules in the mutant active site. The presence of water molecules in the mutant active site is consistent
20 with the observation that TEAS W273S gives rise to multiple hydroxylated terpenoid reaction products.

 The FHP electron density in each W273S crystal structure was sufficient to suggest that FHP existed in a more extended conformation in the W273S structure, compared to the more tightly folded conformation of FHP in the wild-type
25 TEAS/FHP complex. The observation that the active site of W273S binds multiple conformations of FHP is consistent with the fact that W273S converts FPP to multiple terpenoid hydrocarbon products.

TEAS C440W / W273S: TEAS C440W / W273S crystallized under conditions identical to wild-type TEAS. A 0.3 mm crystal was soaked for 20 minutes
30 in reservoir solution saturated in farnesyl hydroxy phosphate (FHP). After cryoprotection and flash freezing as described for wild-type TEAS, data were collected on a laboratory source with Cu-K α radiation (MacScience Corp., Japan). A starting model of uncomplexed TEAS (Table 11) (Brookhaven Protein Database Code 5EAT (PDB 5EAT), with waters and magnesiums removed, was positioned
35 against the mutant data with the rigid body module of the software program X-PLOR (A.T. Brunge, X-PLOR Version 3.1 – A System for X-Ray Crystallography and NMR Yale University Press, New Haven, 1992, pp. 187-207). Rounds of positional and

restrained b-factor refinement with bulk solvent modeling were also carried out in X-PLOR, with manual model building and adjustment carried out in the software program O (Jones, TA, Zou, JY, Cowan, SW, and Kjeldgaard, M., Acta Cryst. D., 49:148-157, 1993). Additional rounds of refinement and map calculation using the
5 CNS program suite resulted in significantly improved maps; this improvement was likely due to improved bulk solvent modeling.

TEAS C440W: TEAS C440W crystallized under conditions identical to wild-type TEAS, except that crystals nucleated less readily and were generally smaller. A mutant crystal was soaked for 6 hours in reservoir solution saturated in
10 FHP before flash-freezing and data collection at SSRL beamline 7-1 (Stanford Synchrotron Radiation Laboratory, Menlo Park, California). A starting model of TEAS-FHP (Table 10), with water molecules, ligands, and residues 523-532 of SEQ ID NO:2 removed, was positioned against the data with the rigid body module of X-PLOR. Rounds of positional and restrained b-factor refinement with bulk solvent and
15 overall anisotropic temperature factor modeling were also carried out in X-PLOR, and manual model building and adjustment were carried out in the software program O. As with the double mutant, electron density maps were noticeably improved after refinement and map calculation in CNS.

20

EXAMPLE 4

TERPENE SYNTHASE ENZYME ASSAYS

Synthase activity assays were carried out based on the assay
25 described in Vogeli and Chappell, Plant Physiol. 94:1860 (1990) and Vogeli, et al., Plant Physiol. 93:182 (1990). In general, radio-labeled (^3H or ^{14}C) substrate was incubated with enzyme at room temperature in a buffered magnesium salt solution (200 mM Tris, pH 8, 50 mM Mg chloride, 1mM DTT, unless otherwise noted); hydrocarbon products were then selectively extracted into an organic solvent such as
30 hexane. The hexane extract generally was treated with silica gel to remove prenyl alcohols and other oxygenated compounds generated by non-enzymatic hydrolysis of substrate, which partition inefficiently into hexane. Hydrocarbon products present in the hexane phase were quantitated by scintillation counting.

A subsequent extraction with a more polar organic solvent such as
35 ethyl acetate was sometimes carried out. Oxygenated compounds more efficiently partition into ethyl acetate-type solvents. Compounds present in the ethyl acetate phase were also quantitated by scintillation counting.

Substrate concentrations typically ranged from 0.1 nanomolar to 100 micromolar. In some assays, the substrate was not radiolabeled. Reactions generally were carried out in triplicate for each substrate concentration. Protein concentration was determined by the Bradford method. For determination of steady-state kinetic parameters, enzyme concentrations were chosen such that generation of products over time was linear throughout the course of the reaction.

Diterpene synthase assays typically were carried out using ^3H geranylgeranyl diphosphate (GGPP) and enzyme in 250 mM Tris, 10 mM Mg chloride, 1mM DTT, pH 8.0. Sesquiterpene synthase assays typically were carried out using ^{14}C or ^3H FPP and enzyme in 100mM Tris, 30 mM Mg chloride, 1 mM DTT, pH 8.0. Monoterpene synthase assays typically were carried out using ^3H GPP and enzyme. As a control for nonspecific binding of GPP by protein, identical reactions were set up which contained BSA, rather than enzyme.

Product analysis of wild type and mutant TEAS enzymes by Ag-TLC. Terpenoid hydrocarbon products are not readily separated by thin layer chromatography on normal or reverse-phase plates; however, some can be separated by argentation TLC (Ag-TLC), in which silica plates are first treated with silver nitrate. Ag-TLC described here generally followed the procedure described by Back et al., Arch. Biochem. Biophys. 315:527 (1994). A silica TLC plate was dipped in 15% silver nitrate (aqueous), then dried for 3-5 hours at 110°C. After spotting of tritiated enzymatic products (solvent extract), the plate was developed in benzene:hexane, ethyl acetate (50:50:1, by volume), sprayed with En 3 Hance (NEN) fluorography spray, placed on film, and exposed for several days to several weeks. Long exposure times were generally necessary, as silver-nitrate treatment of the TLC plate appeared to cause quenching of the fluorography reagent's fluorescence. Alternatively, ^{14}C labelled products were detected after one to two days without the use of fluorography spray.

30

EXAMPLE 5

ACTIVITY OF TEAS W273S

Diterpene Synthase Activity of TEAS W273S. The TEAS W273S enzyme and radiolabelled GGPP were incubated as described above and hydrocarbon products were extracted with hexane. Oxygenated products were then extracted with ethyl acetate. Reactions using wild-type TEAS gave counts lower than buffer alone. TEAS W273S, on the other hand, gave counts that were significantly

higher for both the hexane and ethyl acetate extracts. Hydrocarbon products formed from GGPP by W273S were distinct from the products made by acid-catalyzed loss of diphosphates from GGPP. See Figure 3.

Sesquiterpene Synthase Activity of TEAS W273S. Products of FPP turnover by the purified TEAS W273S mutant were analyzed by argentation thin-layer chromatography (Ag-TLC). One major reaction product had an R_f of 0.7 by Ag-TLC, which was distinct from both 5-epi-aristolochene ($R_f = 0.78$) and vetispiradiene ($R_f = 0.63$). See Figure 4. Preliminary GC/MS data showed that hexane extracts from FPP turnover by TEAS W273S contained at least four terpene hydrocarbons, with mass spectra distinct from either 5-epi-aristolochene or vetispiradiene. One of these products had a mass spectrum similar to germacrene A.

15

EXAMPLE 6

ACTIVITY OF TEAS C440W/W273S

Diterpene Synthase Activity of TEAS C440W/W273S. The mutant TEAS C440W/W273S protein contains a tryptophan residue at position 440 and a serine residue at position 273. Assays with GGPP were carried out using 0.5 micromolar ^3H GGPP, various concentrations of unlabelled GGPP (Echelon), and enzyme. Reactions were incubated for 60 minutes at room temperature. The TEAS C440W/W273S mutant protein converted GGPP to hexane-extractable products, whereas the wild-type enzyme did not. The results indicated that the product profile was altered compared to wild-type TEAS. Hexane-extractable products of GGPP turnover by the double mutant were analyzed by Ag-TLC. The products included two species ($R_f = 0.11$ and 0.28) that were distinct from the hydrolysis product geranylgeraniol ($R_f = 0.0$). To verify that products generated by TEAS C440W/W273S from GGPP were not the hydrolysis product, geranylgeraniol, a sample was analyzed by Ag-TLC. A reaction containing ^3H GGPP ($5\mu\text{m}$) and enzyme ($40\mu\text{m}$) in 100 microliters buffer was incubated overnight at room temperature. As controls, ^3H GGPP was incubated in reaction buffer alone and in reaction buffer adjusted to pH 1.5. Both the enzymatic and control reactions were extracted with hexane, which was spotted on an argentation TLC plate, and developed and exposed as described above. The results, shown in Figure 3, demonstrated that the products formed by TEAS C440W/W273S were different from those generated by non-enzymatic degradation of geranylgeranyl diphosphate.

Sesquiterpene Synthase Activity of TEAS C440W/W273S.

Reactions with FPP as substrate were carried out with ^{14}C FPP ($9\mu\text{M}$) and enzyme ($160\mu\text{M}$) in reaction buffer ($20\mu\text{l}$). After incubating for 30 minutes at room temperature, products made by TEAS C440W / W273S were analyzed by Ag-TLC.

- 5 The product profile of the double mutant was similar to that of TEAS W273S, with the addition of a major product having an R_f of 0.57. The new product was distinct from both 5-*epi*-aristolochene and vetispiradiene. Several other products were also formed, many of which migrated slowly upon argentation TLC. See Fig. 4.

10

EXAMPLE 7
ACTIVITY OF TEAS C440W

- Diterpene Synthase Activity of TEAS C440W.** Enzyme assays
15 with TEAS C440W were carried out as described in Example 6. As shown in Fig. 3, no hexane-extractable products were detectable by Ag-TLC after an overnight incubation at room temperature with $160\mu\text{M}$ of enzyme and $9\mu\text{M}$ radiolabeled GGPP in $20\mu\text{l}$ volume.

- Sesquiterpene Synthase Activity of TEAS C440W.** Ag-TLC
20 analysis of the products made from radiolabelled by purified TEAS C440W detected the formation at least one major terpenoid hydrocarbon product (R_f 0.63) that was distinct from 5-*epi*-aristolochene (R_f 0.78) and vetispiradiene. The reactions product profile on Ag-TLC is shown in Fig. 4. Small amounts of slowly-migrating products (R_f 0-0.09) were also formed.

- 25 **GC/MS analysis of the hexane extract of TEAS C440W terpenoid hydrocarbon reaction products** confirmed that this mutant formed a single major sesquiterpene hydrocarbon product as well as a small number of minor hydroxylated products. The mass spectrum of the major product closely matched the published mass spectrum of the spirocyclic compound hinesene. Hinesene differs from
30 vetispiradiene in the stereochemistry at the C3 methyl group.

EXAMPLE 8**ACTIVITY OF TEAS W273E**

5 **Sesquiterpene Synthase Activity of TEAS W273E.** Reactions to determine the products made by TEAS W273E using FPP as substrate were carried out essentially as described above, using radiolabeled FPP. The results indicated that at least one product other than 5-*epi*-aristolochene was formed. The results also indicated that alkylation of TEAS by FPP had occurred. The alkylation was
10 dependent upon the presence of MgCl₂ in the reaction mixture. In control experiments, boiled W273E-TEAS, as well as wild-type TEAS and BSA, were not alkylated. These results indicate that alkylation had occurred at position 273 and that the amino acid residue at position 273 is part of the active site.

15

EXAMPLE 9**ACTIVITY OF TEAS Y520F**

Sesquiterpene Synthase Activity of TEAS Y520F. Reactions with
20 radiolabeled FPP and TEAS Y520F enzyme were carried out essentially as described above. Reaction products were analysed by Ag-TLC and by GC/MS. A major product of the TEAS Y520F reaction had the same GC retention time as authentic germacrene A and the same mass spectrum as authentic germacrene A. The retention time and mass spectrum of this product were different from 5-*epi*-
25 aristolochene.

EXAMPLE 10**ACTIVITY OF TEAS Y527F**

30 **Enzymatic Activity of TEAS Y527F.** A crude extract of TEAS Y527F enzyme was made by inducing expression in *E. coli* cells, and sonicating the cells. The sonicate was clarified and the supernatant used for enzyme assays. No products were observed in assays using GPP as a substrate, indicating that TEAS Y527F does not have monoterpene synthase activity. Reaction products were
35 obtained using FPP as a substrate. Analysis of these products by Ag-TLC indicated that products other than 5-*epi*-aristolochene were generated by the TEAS Y527F enzyme.

EXAMPLE 11

ALIGNMENT OF TERPENE SYNTHASE SEQUENCES

5

Residues 265 to 535 of the TEAS primary amino acid sequence (SEQ ID NO: 2) were aligned with the full-length amino acid sequence of a limonene synthase (SEQ ID NO: 22), using the BLASTp program (NCBI) with a BLOSUM 62 scoring matrix, a gap open value of 11, a gap extension value of 1, an x_dropoff value of 50, an expect value of 10, a wordsize of 3 and no filtering of low complexity sequences. The output of the alignment program, shown in Table 12, included a gap between residues 527 and 528 of the TEAS sequence (numbered as 263 and 264 in the alignment output). Residues 321, 324, 345, 348, 349, 427, 452, 453, 454, 455, 458, 492, 496, 569, 572, 573, 577, 579 and 580 were selected as having the most suitable alignment with the 19 TEAS residues. Residue 580 of limonene cyclase instead of residue 583 was selected as aligning with residue 528 of TEAS, in order to maintain the spatial orientation of structural aspects found in TEAS, i.e., α -helices, β -sheets and loops shown in Figure 1 and Table 10.

A region including residues 579 to 847 of the taxadiene primary amino acid sequence of SEQ ID NO: 44 was aligned with the full-length amino acid sequence of a bornyl diphosphate synthase (SEQ ID NO: 26), using the BLASTp program (NCBI) with a BLOSUM 62 scoring matrix, a gap open value of 11, a gap extension value of 1, an x_dropoff value of 50, an expect value of 10, a wordsize of 3 and no filtering of low complexity sequences. The output of the alignment program, shown in Table 13, included a gap between residues 453 and 454 of the bornyl diphosphate synthase sequence. Residues 321, 324, 344, 347, 348, 426, 451, 452, 453, 454, 457, 492, 496, 568, 571, 572, 576, 578 and 579 of the bornyl diphosphate synthase were selected as having the most suitable alignment with residues 584, 587, 606, 609, 610, 688, 713, 714, 715, 716, 719, 753, 757, 831, 834, 835, 839, 841 and 842 of the query region sequence of SEQ ID NO: 44. Residues 453 and 454 of bornyl diphosphate synthase were selected to align with residues 715 and 716 of taxadiene synthase, in order to maintain the spatial orientation of structural aspects expected to be present in taxadiene synthase, i.e., α -helices, β -sheets and loops shown in Figure 1 and Table 10.

Residues 265 to 535 of the TEAS primary amino acid sequence (SEQ ID NO: 2) were aligned with the full-length amino acid sequence of a δ -selinene

synthase (SEQ ID NO: 48), using the BLASTp program (NCBI) with a BLOSUM 50 scoring matrix, a gap open value of 13, a gap extension value of 2, an x_dropoff value of 50, an expect value of 10, a wordsize of 3 and no filtering of low complexity sequences. The output of the alignment program is shown in Table 14. Residues
 5 300, 303, 324, 327, 328, 406, 431, 432, 433, 434, 437, 471, 475, 548, 551, 552, 556, 558 and 559 of SEQ ID NO:48 were selected as having the most suitable alignment with residues 270, 273, 294, 297, 298, 376, 401, 402, 403, 404, 407, 440, 444, 516, 519, 520, 525, 527 and 528 of SEQ ID NO: 2.

Residues 307 to 593 of the primary amino acid sequence of γ -
 10 humulene synthase (SEQ ID NO: 50) were aligned with the full-length amino acid sequence of abietadiene synthase (SEQ ID NO: 56), using the BLASTp program (NCBI) with a BLOSUM 62 scoring matrix, a gap open value of 11, a gap extension value of 1, an x_dropoff value of 50, an expect value of 10, a wordsize of 3 and no filtering of low complexity sequences. The output of the alignment program is shown
 15 in Table 15. Residues 590, 593, 614, 617, 618, 696, 721, 722, 723, 724, 727, 761, 765, 837, 840, 841, 845, 847 and 848 of the diterpene synthase (SEQ ID NO: 56) were selected as having the most suitable alignment with residues 312, 315, 336, 339, 340, 419, 444, 445, 446, 447, 450, 484, 488, 562, 565, 566, 570, 572 and 573 of the sesquiterpene synthase query sequence (SEQ ID NO: 50).

20

EXAMPLE 12

GENERATION OF NOVEL MONOTERPENE SYNTHASE GENES

25 A DNA sequence encoding a pinene synthase (SEQ ID NO:20) is used to construct a library of mutant pinene synthase genes. Random mutations are introduced at nucleotides encoding one or more of the following nine amino acid residues: L, C, C, G, H, S, L, G and Y, which correspond to positions 351, 372, 480, 481, 482, 485, 519, 600 and 601 of SEQ ID NO:20.

30 In some cases, the pinene synthase coding sequence is randomly mutated at nucleotides encoding one or more of amino acid residues 348, 375, 376, 597, 605, 607 and 608, which correspond to positions Y, I, T, F, D, Y and S of SEQ ID NO:20. The pinene synthase coding sequence is sometimes mutated at nucleotides encoding one or more of the following amino acid residues: Y, S and G,
 35 which correspond to positions 454, 479 and 523 of SEQ ID NO:20. In some cases, mutations at these ten positions are made in addition to mutations at nucleotides encoding the nine residues mentioned above. In other cases, mutations at these ten

positions are made without introducing mutations at the nine residues mentioned above.

5 The pinene synthase coding sequence DNA is inserted in the pET28b(+) vector and mutagenized using the QuickChange® method, following a protocol similar to that described in Example 1 for the TEAS 406/407 random library. The primers used to generate mutations are synthesized as indicated in Example 1, using N or S as nucleotides in the desired codons in order to generate random mutants.

10 Specific mutations at one or more of the above 19 pinene synthase amino acid residues are made by site-directed mutagenesis using a protocol similar to that described in Example 1 for TEAS. Primers are made that have specific A, T, C or G substitutions in the codons to be mutated, in order to generate the desired mutant(s).

15 Random and/or specific mutations are prepared in a manner similar to that described above to alter amino acid residues of other monoterpene synthases, e.g., limonene synthase, (SEQ ID NOS:22 or 58), myrcene synthase (SEQ ID NO:30), α -sabinene synthase (SEQ ID NO:54), 1, 8 cineole synthase (SEQ ID NO:24) and α -bornyl diphosphate synthase (SEQ ID NO:26), at residues whose α -carbons have the interatomic distances and structural coordinates described in Tables 1-6.

20

EXAMPLE 13

GENERATION OF NOVEL SESQUITERPENE SYNTHASE GENES

25 A DNA sequence encoding a cadinene synthase (SEQ ID NO:33) is used to construct a library of mutant cadinene synthases. Random mutations are introduced at nucleotides encoding one or more of the following nine amino acid residues: W, I, S, G, Y, L, C, L and Y, which correspond to amino acid residues 280, 301, 409, 410, 411, 414, 448, 527 and 528 encoded by SEQ ID NO:33.

30 In some cases, the cadinene synthase coding sequence is mutated at nucleotides encoding one or more of amino acid residues G, A, S, M, D, Y and T, which correspond to amino acid residues 277, 304, 305, 524, 532, 534 and 535 encoded by SEQ ID NO:33. In addition, the cadinene synthase coding sequence is sometimes mutated at nucleotides encoding one or more of the following amino acid
35 residues: 383, 408 and 452, which correspond to amino acids Y, T and D encoded by SEQ ID NO:33. In some cases, these mutations are made in addition to mutations at the nine residues mentioned above. In other cases, mutations at these

ten residues are made without introducing mutations at the nine residues mentioned above.

The cadinene synthase coding sequence is mutated using the QuickChange® method in the pET28b(+) vector, following a protocol similar to that described in Example 1 for the TEAS 406/407 random library. The primers used to generate mutations are synthesized as indicated in Example 11.

Specific mutations at one or more of the above cadinene synthase amino acid residues are made by site-directed mutagenesis using a protocol similar to that described in Example 1 for TEAS.

Random and/or specific mutations are prepared in a manner similar to that described above to alter amino acid residues of other sesquiterpene synthases, e.g., vetispiradiene synthase (SEQ ID NO:32), germacrene C synthase (SEQ ID NO:52), E-alpha-bisabolene synthase (SEQ ID NO:46), gamma-humulene synthase (SEQ ID NO:50), delta-selinene synthase (SEQ ID NO:48), e-b-farnesene synthase (SEQ ID NO:28), at residues whose α -carbons have the interatomic distances and structural coordinates described in Tables 1-6.

EXAMPLE 14

GENERATION OF NOVEL DITERPENE SYNTHASE GENES

A DNA sequence encoding an abietadiene synthase (SEQ ID NO:56) is used to construct a library of mutant abietadiene synthases. Random mutations are introduced at nucleotides encoding one or more of the following nine amino acid residues: S, S, I, A, L, V, G, F and Y, which correspond to positions 593, 614, 722, 723, 724, 727, 761, 840 and 841 of SEQ ID NO:56.

In some cases, the abietadiene synthase coding sequence is mutated at nucleotides encoding one or more of amino acid residues I, S, T, M, D, L and T, which correspond to positions 590, 617, 618, 837, 845, 847 and 848 of SEQ ID NO:56. The abietadiene synthase coding sequence is sometimes mutated at nucleotides encoding one or more of the following amino acid residues: Y, S and N, which correspond to positions 696, 721 and 765 of SEQ ID NO:56. In some cases, these mutations are made in addition to mutations at the nine residues mentioned above. In other cases, mutations are made at these ten residues without introducing mutations at the nine residues mentioned above.

The abietadiene synthase coding sequence is mutated using the QuickChange® method in the pET28b(+) vector, following a protocol similar to that

described in Example 1 for the TEAS 406/407 random library. The primers used to generate mutations are synthesized as indicated in Example 11.

Specific mutations at one or more of the above abietadiene synthase amino acid residues are made by site-directed mutagenesis using a protocol similar to that described in Example 1 for TEAS.

Random and/or specific mutations are prepared in a manner similar to that described above to alter amino acid residues of other diterpene synthases at amino acid residues whose α -carbons have the interatomic distances and structural coordinates described in Tables 1-6, e.g., casbene synthase (SEQ ID NO:42) and taxadiene synthase (SEQ ID NO:44).

EXAMPLE 15

EXPRESSION OF MUTANT SYNTHASES IN INSECT, MAMMALIAN AND BACTERIAL CELLS

Constructs containing nucleic acids encoding mutant synthases of Examples 12, 13 and/or 14 are introduced into cultured cells of the insect *Spodoptera frugiperda* using a baculovirus expression vector. After expression of the gene, the mutant enzyme is isolated and purified from each clone.

Constructs containing nucleic acids encoding mutant synthases of Examples 12, 13 and/or 14 are introduced into cultured HeLa cells using an expression vector having an SV40 promoter. After expression of the gene, the mutant enzyme is isolated and purified from each clone.

Constructs containing nucleic acids encoding mutant synthases of Examples 12, 13 and/or 14 are introduced into *E. coli* BL-21 on a plasmid vector as described in Example 1. The mutant synthase gene is expressed and the mutant enzyme is isolated and purified as described in Example 2.

OTHER EMBODIMENTS

To the extent not already indicated, it will be understood by those of ordinary skill in the art that any one of the various specific embodiments herein described and illustrated may be further modified to incorporate features shown in other of the specific embodiments.

It is to be understood that while the invention has been described in conjunction with the Detailed Description thereof, that the foregoing description is

intended to illustrate, and not limit the scope of the invention, which is defined by the scope of the appended claims. Other aspects, advantages, and modifications are within the scope of the following claims.

Table 1

| α - Carbon | X Position | Y Position | Z Position |
|----------------------|---------------|---------------|---------------|
| 1 | 119.144 | 43.487 | 44.133 |
| 2 | 120.203 | 38.695 | 43.506 |
| 3 | 114.058 | 43.884 | 41.015 |
| 4 | 109.327 | 46.145 | 41.743 |
| 5 | 110.682 | 46.410 | 45.284 |
| 6 | 99.381 | 42.920 | 45.148 |
| 7 | 103.445 | 38.054 | 44.605 |
| 8 | 106.807 | 36.336 | 45.151 |
| 9 | 107.629 | 38.010 | 41.804 |
| 10 | 109.375 | 34.842 | 40.617 |
| 11 | 111.944 | 37.854 | 37.602 |
| 12 | 110.233 | 31.098 | 47.361 |
| 13 | 109.178 | 33.314 | 52.875 |
| 14 | 115.915 | 32.218 | 48.369 |
| 15 | 118.846 | 34.443 | 51.796 |
| 16 | 116.461 | 32.848 | 54.290 |
| 17 | 114.100 | 38.006 | 55.620 |
| 18 | 116.617 | 41.285 | 51.702 |
| 19 | 114.855 | 43.486 | 54.238 |

Table 2

| α -carbon | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 |
|------------------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| 1 | 0.0 | 5.0 | 6.0 | 10.5 | 9.0 | 19.8 | 16.6 | 14.3 | 13.0 | 13.5 | 11.2 | 15.6 | 16.7 | 12.5 | 11.8 | 15.0 | 13.7 | 8.3 | 11.0 |
| 2 | 5.0 | 0.0 | 8.4 | 13.3 | 12.4 | 21.3 | 16.8 | 13.7 | 12.7 | 11.9 | 10.2 | 13.1 | 15.4 | 9.2 | 9.4 | 12.8 | 13.6 | 9.3 | 12.9 |
| 3 | 6.0 | 8.4 | 0.0 | 5.3 | 6.0 | 15.3 | 12.6 | 11.3 | 8.7 | 10.2 | 7.2 | 14.8 | 16.6 | 13.9 | 15.1 | 17.4 | 15.7 | 11.3 | 13.3 |
| 4 | 10.5 | 13.3 | 5.3 | 0.0 | 3.8 | 11.0 | 10.4 | 10.7 | 8.3 | 11.4 | 9.6 | 16.1 | 17.0 | 16.8 | 18.1 | 19.6 | 16.8 | 13.3 | 13.9 |
| 5 | 9.0 | 12.4 | 6.0 | 3.8 | 0.0 | 11.8 | 11.1 | 10.8 | 9.6 | 12.5 | 11.6 | 15.5 | 15.2 | 15.4 | 15.9 | 17.3 | 13.8 | 10.1 | 10.3 |
| 6 | 19.8 | 21.3 | 15.3 | 11.0 | 11.8 | 0.0 | 6.4 | 9.9 | 10.2 | 13.6 | 15.5 | 16.2 | 15.8 | 20.0 | 22.2 | 21.8 | 18.7 | 18.5 | 18.0 |
| 7 | 16.6 | 16.8 | 12.6 | 10.4 | 11.1 | 6.4 | 0.0 | 3.8 | 5.0 | 7.8 | 11.0 | 10.1 | 11.1 | 14.3 | 17.4 | 17.0 | 15.3 | 15.3 | 15.9 |
| 8 | 14.3 | 13.7 | 11.3 | 10.7 | 10.8 | 9.9 | 3.8 | 0.0 | 3.8 | 5.4 | 9.3 | 6.6 | 8.6 | 10.5 | 13.9 | 13.7 | 12.9 | 12.8 | 14.1 |
| 9 | 13.0 | 12.7 | 8.7 | 8.3 | 9.8 | 10.2 | 5.0 | 3.8 | 0.0 | 3.8 | 6.0 | 9.2 | 12.1 | 12.1 | 15.4 | 16.1 | 15.3 | 13.8 | 15.4 |
| 10 | 13.5 | 11.9 | 10.2 | 11.4 | 12.5 | 13.6 | 7.8 | 5.4 | 3.8 | 0.0 | 5.0 | 7.8 | 12.4 | 10.5 | 14.6 | 15.5 | 16.0 | 14.7 | 17.0 |
| 11 | 11.2 | 10.2 | 7.2 | 9.6 | 11.6 | 15.5 | 11.0 | 9.3 | 6.0 | 5.0 | 0.0 | 12.0 | 16.2 | 12.8 | 16.1 | 18.0 | 18.2 | 15.3 | 17.8 |
| 12 | 15.6 | 13.1 | 14.8 | 16.1 | 15.5 | 16.2 | 10.1 | 6.6 | 9.2 | 7.8 | 12.0 | 0.0 | 6.0 | 5.9 | 10.2 | 9.5 | 11.4 | 12.8 | 14.9 |
| 13 | 16.7 | 15.4 | 16.6 | 17.0 | 15.2 | 15.8 | 11.1 | 8.6 | 12.1 | 12.4 | 16.2 | 6.0 | 0.0 | 8.2 | 9.8 | 7.4 | 7.3 | 11.0 | 11.7 |
| 14 | 12.5 | 9.2 | 13.9 | 16.8 | 15.4 | 20.0 | 14.3 | 10.5 | 12.1 | 10.5 | 12.8 | 5.9 | 8.2 | 0.0 | 5.0 | 6.0 | 9.5 | 9.7 | 12.8 |
| 15 | 11.8 | 9.4 | 15.1 | 18.1 | 15.9 | 22.2 | 17.4 | 13.9 | 15.4 | 14.8 | 16.1 | 10.2 | 9.8 | 5.0 | 0.0 | 3.8 | 7.1 | 7.2 | 10.2 |
| 16 | 15.0 | 12.8 | 17.4 | 19.6 | 17.3 | 21.8 | 17.0 | 13.7 | 16.1 | 15.5 | 18.0 | 9.5 | 7.4 | 6.0 | 3.8 | 0.0 | 5.8 | 8.8 | 10.8 |
| 17 | 13.7 | 13.6 | 15.7 | 16.8 | 13.8 | 18.7 | 15.3 | 12.9 | 15.3 | 16.0 | 18.2 | 11.4 | 7.3 | 9.5 | 7.1 | 5.8 | 0.0 | 5.7 | 5.7 |
| 18 | 8.3 | 9.3 | 11.3 | 13.3 | 10.1 | 18.5 | 15.3 | 12.8 | 13.8 | 14.7 | 15.3 | 12.8 | 11.0 | 9.7 | 7.2 | 8.8 | 5.7 | 0.0 | 3.8 |
| 19 | 11.0 | 12.9 | 13.3 | 13.9 | 10.3 | 18.0 | 15.9 | 14.1 | 15.4 | 17.0 | 17.8 | 14.9 | 11.7 | 12.8 | 10.2 | 10.8 | 5.7 | 3.8 | 0.0 |

Table 3

| α - Carbon | X Position | Y Position | Z Position |
|----------------------|---------------|---------------|---------------|
| 1 | 119.144 | 43.487 | 44.133 |
| 2 | 120.203 | 38.695 | 43.506 |
| 3 | 114.058 | 43.884 | 41.015 |
| 4 | 109.327 | 46.145 | 41.743 |
| 5 | 110.682 | 46.410 | 45.284 |
| 6 | 106.807 | 36.336 | 45.151 |
| 7 | 107.629 | 38.010 | 41.804 |
| 8 | 109.375 | 34.842 | 40.617 |
| 9 | 111.944 | 37.854 | 37.602 |
| 10 | 110.233 | 31.098 | 47.361 |
| 11 | 115.915 | 32.218 | 48.369 |
| 12 | 118.846 | 34.443 | 51.796 |
| 13 | 116.461 | 32.848 | 54.290 |
| 14 | 114.100 | 38.006 | 55.620 |
| 15 | 116.617 | 41.285 | 51.702 |
| 16 | 114.855 | 43.486 | 54.238 |

Table 4

| α -Carbon | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 |
|------------------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| 1 | 0.0 | 5.0 | 6.0 | 10.5 | 9.0 | 14.3 | 13.0 | 13.5 | 11.2 | 15.6 | 12.5 | 11.8 | 15.0 |
| 2 | 5.0 | 0.0 | 8.4 | 13.3 | 12.4 | 13.7 | 12.7 | 11.9 | 10.2 | 13.1 | 9.2 | 9.4 | 12.8 |
| 3 | 6.0 | 8.4 | 0.0 | 5.3 | 6.0 | 11.3 | 8.7 | 10.2 | 7.2 | 14.8 | 13.9 | 15.1 | 17.4 |
| 4 | 10.5 | 13.3 | 5.3 | 0.0 | 3.8 | 10.7 | 8.3 | 11.4 | 9.6 | 16.1 | 16.8 | 18.1 | 19.6 |
| 5 | 9.0 | 12.4 | 6.0 | 3.8 | 0.0 | 10.8 | 9.6 | 12.5 | 11.6 | 15.5 | 15.4 | 15.9 | 17.3 |
| 6 | 14.3 | 13.7 | 11.3 | 10.7 | 10.8 | 0.0 | 3.8 | 5.4 | 9.3 | 6.6 | 10.5 | 13.9 | 13.7 |
| 7 | 13.0 | 12.7 | 8.7 | 8.3 | 9.6 | 3.8 | 0.0 | 3.8 | 6.0 | 9.2 | 12.1 | 15.4 | 16.1 |
| 8 | 13.5 | 11.9 | 10.2 | 11.4 | 12.5 | 5.4 | 3.8 | 0.0 | 5.0 | 7.8 | 10.5 | 14.6 | 15.5 |
| 9 | 11.2 | 10.2 | 7.2 | 9.6 | 11.6 | 9.3 | 6.0 | 5.0 | 0.0 | 12.0 | 12.8 | 16.1 | 18.0 |
| 10 | 15.6 | 13.1 | 14.8 | 16.1 | 15.5 | 6.6 | 9.2 | 7.8 | 12.0 | 0.0 | 5.9 | 10.2 | 9.5 |
| 11 | 12.5 | 9.2 | 13.9 | 16.8 | 15.4 | 10.5 | 12.1 | 10.5 | 12.8 | 5.9 | 0.0 | 5.0 | 6.0 |
| 12 | 11.8 | 9.4 | 15.1 | 18.1 | 15.9 | 13.9 | 15.4 | 14.6 | 16.1 | 12.2 | 5.0 | 0.0 | 3.8 |
| 13 | 15.0 | 12.8 | 17.4 | 19.6 | 17.3 | 13.7 | 16.1 | 15.5 | 18.0 | 9.5 | 6.0 | 3.8 | 0.0 |
| 14 | 13.7 | 13.6 | 15.7 | 16.8 | 13.8 | 12.9 | 15.3 | 16.0 | 18.2 | 11.4 | 9.5 | 7.1 | 5.8 |
| 15 | 8.3 | 9.3 | 11.3 | 13.3 | 10.1 | 12.8 | 13.8 | 14.7 | 15.3 | 12.8 | 9.7 | 7.2 | 8.8 |
| 16 | 11.0 | 12.9 | 13.3 | 13.9 | 10.3 | 14.1 | 15.4 | 17.0 | 17.8 | 14.9 | 12.8 | 10.2 | 10.8 |

Table 4

| α -Carbon | 14 | 15 | 16 |
|------------------|------|------|------|
| 1 | 13.7 | 8.3 | 11.0 |
| 2 | 13.6 | 9.3 | 12.9 |
| 3 | 15.7 | 11.3 | 13.3 |
| 4 | 16.8 | 13.3 | 13.9 |
| 5 | 13.8 | 10.1 | 10.3 |
| 6 | 12.9 | 12.8 | 14.1 |
| 7 | 15.3 | 13.8 | 15.4 |
| 8 | 16.0 | 14.7 | 17.0 |
| 9 | 18.2 | 15.3 | 17.8 |
| 10 | 11.4 | 12.8 | 14.9 |
| 11 | 9.5 | 9.7 | 12.8 |
| 12 | 7.1 | 7.2 | 10.2 |
| 13 | 5.8 | 8.8 | 10.8 |
| 14 | 0.0 | 5.7 | 5.7 |
| 15 | 5.7 | 0.0 | 3.8 |
| 16 | 5.7 | 3.8 | 0.0 |

Table 5

| α - Carbon | X Position | Y Position | Z Position |
|----------------------|---------------|---------------|---------------|
| 1 | 120.203 | 38.695 | 43.506 |
| 2 | 114.058 | 43.884 | 41.015 |
| 3 | 106.807 | 36.336 | 45.151 |
| 4 | 107.629 | 38.010 | 41.804 |
| 5 | 109.375 | 34.842 | 40.617 |
| 6 | 111.944 | 37.854 | 37.602 |
| 7 | 110.233 | 31.098 | 47.361 |
| 8 | 118.846 | 34.443 | 51.796 |
| 9 | 116.461 | 32.848 | 54.290 |

Table 6

| α -Carbon | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 |
|------------------|------|------|------|------|------|------|------|------|------|
| 1 | 0 | 8.4 | 13.7 | 12.7 | 11.9 | 10.2 | 13.1 | 9.4 | 12.8 |
| 2 | 8.4 | 0 | 11.3 | 8.7 | 10.2 | 7.2 | 14.8 | 15.1 | 17.4 |
| 3 | 13.7 | 11.3 | 0 | 3.8 | 5.4 | 9.3 | 6.6 | 13.9 | 13.7 |
| 4 | 12.7 | 8.7 | 3.8 | 0 | 3.8 | 6 | 9.2 | 15.4 | 16.1 |
| 5 | 11.9 | 10.2 | 5.4 | 3.8 | 0 | 5 | 7.8 | 14.6 | 15.5 |
| 6 | 10.2 | 7.2 | 9.3 | 6 | 5 | 0 | 12 | 16.1 | 18 |
| 7 | 13.1 | 14.8 | 6.6 | 9.2 | 7.8 | 12 | 0 | 10.2 | 9.5 |
| 8 | 9.4 | 15.1 | 13.9 | 15.4 | 14.6 | 16.1 | 10.2 | 0 | 3.8 |
| 9 | 12.8 | 17.4 | 13.7 | 16.1 | 15.5 | 18 | 9.5 | 3.8 | 0 |

Table 7

| Ordered Arrangement of R-Groups at α -carbons 1-19 | | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|----|----|----|----|----|----|----|----|----|----|
| | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 |
| A | C | W | I | I | S | Y | T | T | T | Y | L | C | D | V | T | Y | D | Y | T |
| B | C | W | I | I | S | Y | T | S | T | Y | L | C | D | I | T | Y | D | Y | T |
| C | G | W | I | A | S | Y | T | C | G | Y | L | C | D | M | L | Y | D | Y | T |
| D | G | W | I | A | S | Y | T | S | G | Y | L | C | D | M | L | Y | D | Y | T |
| E | C | W | L | T | S | Y | S | A | G | Y | L | A | N | A | Y | Y | D | Y | T |
| F | G | W | L | L | S | Y | S | T | V | H | L | G | D | A | V | Y | D | Y | T |
| G | C | W | L | T | S | Y | S | A | G | Y | L | A | N | A | V | Y | D | Y | T |
| H | L | W | I | T | S | Y | S | V | G | Y | L | A | N | A | V | Y | D | Y | T |
| I | P | W | I | V | D | Y | S | T | A | G | L | F | D | A | C | Y | D | Y | T |
| J | A | W | V | C | G | Y | S | T | C | I | M | S | D | I | T | Y | D | Y | T |
| K | N | F | F | L | G | A | E | I | T | A | T | G | N | I | M | Y | D | Y | T |
| L | C | W | N | I | T | Y | S | I | S | G | L | G | N | V | L | Y | D | Y | T |
| M | S | W | V | L | T | Y | S | S | S | Y | L | G | D | A | S | Y | D | Y | T |
| N | N | F | F | L | V | N | A | T | L | A | L | G | N | L | S | Y | D | Y | T |
| O | C | W | N | I | T | Y | I | S | G | P | L | L | D | A | I | Y | D | Y | T |
| P | C | W | N | V | T | Y | I | S | G | A | L | L | D | A | I | Y | D | Y | T |
| Q | C | Y | L | L | T | F | A | V | T | I | L | L | D | A | I | Y | D | Y | T |
| R | C | W | I | I | T | Y | S | I | S | A | I | L | D | A | I | Y | D | Y | T |
| S | S | W | F | I | V | Y | S | S | S | V | I | L | N | V | I | Y | D | Y | T |
| T | S | W | I | A | T | Y | S | S | A | S | I | L | N | V | I | Y | D | Y | T |
| U | N | W | N | L | T | Y | S | S | S | S | I | L | N | V | I | Y | D | Y | T |
| V | F | L | A | Q | T | Y | S | S | S | Q | L | F | D | A | I | Y | D | Y | T |
| W | I | S | S | T | V | Y | S | S | A | L | V | S | D | A | I | Y | D | Y | T |
| X | Y | L | C | I | T | Y | S | S | G | H | S | L | N | F | I | Y | D | Y | T |
| Y | G | S | F | I | T | F | S | S | S | V | I | L | N | F | I | Y | D | Y | T |
| Z | Y | W | A | C | T | Y | S | S | G | M | L | G | D | L | I | Y | D | Y | T |

Table 7

| | | | | | | | | | | | | | | | | | | | | | |
|----|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| AA | A | A | N | L | T | N | A | L | T | S | T | C | M | L | L | L | Y | D | Y | N | S |
| BB | F | L | C | V | T | Y | S | S | A | Y | V | L | G | D | L | L | Y | D | F | S | S |
| CC | F | W | A | M | T | Y | N | T | G | M | L | L | S | M | M | V | Y | D | Y | T | G |
| DD | Y | M | C | V | T | F | V | S | S | G | S | C | N | G | F | F | Y | D | Y | T | G |
| EE | V | S | G | Q | V | Y | S | A | G | L | V | W | G | V | V | L | Y | D | Y | T | G |
| FF | C | S | G | T | T | M | F | F | A | G | V | G | N | F | L | Y | D | Y | T | G | G |
| GG | C | S | G | T | T | M | S | F | A | L | I | G | N | F | L | Y | D | Y | T | G | G |
| HH | C | A | G | T | T | M | S | F | A | L | I | G | N | F | L | Y | D | Y | T | G | G |
| II | I | W | V | I | S | Y | T | T | G | L | V | I | N | F | L | Y | D | Y | T | G | G |
| JJ | Y | W | A | C | T | Y | S | S | G | M | L | I | D | D | L | Y | D | Y | T | G | G |
| KK | C | W | I | I | S | Y | T | S | T | Y | L | G | D | D | L | Y | D | Y | T | G | G |
| LL | C | W | I | I | S | Y | T | S | T | Y | L | G | D | D | L | Y | D | Y | T | G | G |
| MM | C | W | I | I | T | Y | S | I | S | G | M | L | D | D | L | Y | D | Y | T | G | G |
| NN | F | A | A | Q | T | Y | S | I | G | Q | L | S | D | D | L | Y | D | Y | T | G | G |
| OO | F | A | I | A | T | Y | S | V | A | S | I | L | D | D | L | Y | D | Y | T | G | G |

Table 8

| Ordered Arrangement of R-Groups at α -carbons 1-16 | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|----|----|----|----|----|----|----|
| | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 |
| A | C | W | I | I | S | T | T | Y | L | C | V | T | Y | D | Y | T |
| B | C | W | I | I | S | S | T | Y | L | C | I | T | Y | D | Y | T |
| C | G | W | I | A | S | C | G | Y | L | C | M | L | Y | D | Y | T |
| D | G | W | I | A | S | S | G | Y | L | C | M | L | Y | D | Y | T |
| E | C | W | L | T | S | A | G | Y | L | A | A | L | Y | D | Y | T |
| F | G | W | L | L | S | T | V | H | L | G | A | V | Y | D | Y | T |
| G | C | W | L | T | S | A | G | Y | L | A | A | L | Y | D | Y | T |
| H | L | W | I | T | T | V | G | N | L | F | V | L | Y | D | Y | T |
| I | P | W | I | V | D | T | A | G | L | S | A | C | Y | D | Y | T |
| J | A | W | V | C | G | S | C | I | M | G | A | S | Y | D | Y | T |
| K | N | F | F | L | G | I | T | A | T | G | I | T | Y | D | Y | T |
| L | C | W | N | I | T | I | S | G | M | L | A | M | Y | D | Y | T |
| M | S | W | V | L | T | S | S | Y | L | G | V | L | Y | D | Y | T |
| N | N | F | F | L | V | T | L | A | L | G | L | S | Y | D | Y | T |
| O | C | W | N | I | T | S | G | P | L | L | A | M | Y | D | Y | T |
| P | C | W | N | V | T | G | G | I | L | L | A | I | Y | D | Y | T |
| Q | C | Y | L | L | T | V | T | M | T | G | I | T | Y | D | Y | T |
| R | C | W | I | I | T | I | S | A | I | L | A | I | Y | D | Y | T |
| S | S | W | F | I | V | S | S | V | I | L | V | I | Y | D | Y | T |
| T | S | W | I | A | T | V | S | A | I | L | A | I | Y | D | Y | T |
| U | N | W | N | L | T | I | S | S | I | F | S | M | Y | D | Y | T |
| V | F | L | A | Q | T | I | G | Q | L | S | T | I | F | Y | H | L |
| W | I | S | S | T | V | I | A | L | V | G | M | F | Y | H | L | L |
| X | Y | L | C | I | T | C | G | H | S | L | F | G | Y | H | L | L |
| Y | G | S | F | I | T | S | S | V | I | L | A | V | Y | H | L | L |
| Z | Y | W | A | C | T | S | G | M | L | G | L | I | Y | H | L | L |

Table 8

| | | | | | | | | | | | | | | | | |
|----|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| AA | A | A | L | T | L | T | S | T | C | L | L | L | Y | D | Y | N |
| BB | F | L | V | A | S | T | Y | V | L | L | L | L | Y | D | F | S |
| CC | F | W | M | G | T | T | M | L | S | I | M | I | Y | D | F | S |
| DD | Y | M | V | S | S | T | G | I | L | F | V | V | Y | D | Y | T |
| EE | V | S | Q | G | V | V | L | C | W | V | L | Y | Y | D | Y | G |
| FF | C | S | T | L | A | T | G | V | G | F | L | Y | Y | D | F | T |
| GG | C | S | T | A | A | T | L | I | G | F | L | Y | Y | D | F | T |
| HH | C | A | T | A | A | T | L | I | G | F | L | Y | Y | D | F | T |
| II | I | W | I | G | A | S | L | V | I | T | T | Y | Y | D | F | T |
| JJ | Y | W | C | G | G | T | M | L | G | L | V | Y | Y | D | F | T |
| KK | C | W | I | T | S | S | Y | L | C | I | L | Y | Y | D | F | T |
| LL | C | W | I | T | S | S | Y | L | C | I | L | Y | Y | D | F | T |
| MM | C | W | I | T | S | S | Y | L | C | I | L | Y | Y | D | F | T |
| NN | F | A | N | I | I | I | G | M | C | L | A | Y | F | D | F | T |
| OO | F | A | A | A | V | T | S | L | L | S | T | Y | Y | D | F | T |

Table 9

| Ordered Arrangements of α -Carbons 1-9 | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 |
| A | W | I | T | T | Y | L | C | T | Y |
| B | W | I | S | T | Y | L | C | T | Y |
| C | W | I | C | G | Y | L | C | L | Y |
| D | W | I | S | G | Y | L | C | L | Y |
| E | W | L | A | G | Y | I | A | L | Y |
| F | W | L | T | V | H | L | G | V | Y |
| G | W | L | A | G | Y | I | A | L | Y |
| H | W | I | V | G | N | L | F | L | Y |
| I | W | I | T | A | G | L | S | C | Y |
| J | W | V | S | C | I | M | G | S | Y |
| K | F | F | I | T | A | T | G | T | Y |
| L | W | N | I | S | G | M | L | M | Y |
| M | W | V | S | S | Y | L | G | L | Y |
| N | F | F | T | L | A | L | G | S | Y |
| O | W | N | S | G | P | L | L | M | Y |
| P | W | N | G | G | I | L | L | I | Y |
| Q | Y | L | V | T | M | T | G | T | Y |
| R | W | I | I | S | A | I | L | I | Y |
| S | W | F | S | S | V | I | L | I | Y |
| T | W | I | V | A | S | I | L | I | Y |
| U | W | N | I | S | S | I | F | M | Y |
| V | L | A | I | G | Q | L | S | I | F |
| W | S | S | I | A | L | V | G | F | Y |
| X | L | C | C | G | H | S | L | G | Y |
| Y | S | F | S | S | V | I | L | V | Y |
| Z | W | A | S | G | M | L | G | I | Y |

Table 9

| | | | | | | | | | |
|----|---|---|---|---|---|---|---|---|---|
| AA | A | N | L | T | S | T | C | L | Y |
| BB | L | C | S | A | Y | V | L | L | Y |
| CC | W | A | T | G | M | L | S | M | Y |
| DD | M | C | S | S | G | I | L | V | Y |
| EE | S | G | V | G | L | C | W | F | Y |
| FF | S | G | A | L | G | V | G | F | Y |
| GG | S | G | F | A | L | I | G | F | Y |
| HH | A | G | F | A | L | I | G | F | Y |
| II | W | V | T | G | L | V | I | S | Y |
| JJ | W | A | S | G | M | L | G | I | Y |
| KK | W | I | S | T | Y | L | C | T | Y |
| LL | W | I | T | T | Y | L | C | T | Y |
| MM | W | N | I | S | G | M | L | M | Y |
| NN | A | A | I | G | Q | L | S | I | F |
| OO | A | I | V | A | S | I | L | I | Y |

Table 10
Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase
With Farnesyl Hydroxyphosphonate Bound.

| 5 | Atom | Atom Type | Residue | Residue # | X | Y | Z | OCC | B- factor |
|----|------|--------------|---------|--------------|---------|--------|--------|------|--------------|
| | 1 | CB | VAL | 17 | 105.641 | 55.031 | 61.062 | 1.00 | 98.26 |
| | 2 | CG1 | VAL | 17 | 104.598 | 56.123 | 61.269 | 1.00 | 97.24 |
| 10 | 3 | CG2 | VAL | 17 | 105.492 | 53.957 | 62.133 | 1.00 | 94.24 |
| | 4 | C | VAL | 17 | 106.842 | 53.842 | 59.190 | 1.00 | 98.89 |
| | 5 | O | VAL | 17 | 107.108 | 52.650 | 59.359 | 1.00 | 96.64 |
| | 6 | N | VAL | 17 | 104.381 | 53.419 | 59.594 | 1.00 | 99.88 |
| | 7 | CA | VAL | 17 | 105.495 | 54.412 | 59.646 | 1.00 | 99.06 |
| 15 | 8 | N | ALA | 18 | 107.671 | 54.719 | 58.615 | 1.00 | 98.95 |
| | 9 | CA | ALA | 18 | 109.015 | 54.419 | 58.088 | 1.00 | 98.55 |
| | 10 | CB | ALA | 18 | 110.007 | 55.478 | 58.572 | 1.00 | 97.57 |
| | 11 | C | ALA | 18 | 109.570 | 53.012 | 58.346 | 1.00 | 99.86 |
| | 12 | O | ALA | 18 | 109.580 | 52.170 | 57.447 | 1.00 | 100.00 |
| 20 | 13 | N | ASP | 19 | 110.068 | 52.793 | 59.562 | 1.00 | 99.07 |
| | 14 | CA | ASP | 19 | 110.616 | 51.508 | 60.010 | 1.00 | 97.13 |
| | 15 | CB | ASP | 19 | 109.507 | 50.447 | 60.064 | 1.00 | 96.62 |
| | 16 | CG | ASP | 19 | 109.503 | 49.666 | 61.370 | 1.00 | 97.86 |
| | 17 | OD1 | ASP | 19 | 110.119 | 50.130 | 62.355 | 1.00 | 100.00 |
| 25 | 18 | OD2 | ASP | 19 | 108.873 | 48.588 | 61.415 | 1.00 | 97.98 |
| | 19 | C | ASP | 19 | 111.849 | 50.931 | 59.301 | 1.00 | 95.44 |
| | 20 | O | ASP | 19 | 112.812 | 50.539 | 59.964 | 1.00 | 95.55 |
| | 21 | N | PHE | 20 | 111.814 | 50.854 | 57.971 | 1.00 | 91.33 |
| | 22 | CA | PHE | 20 | 112.925 | 50.297 | 57.190 | 1.00 | 84.17 |
| 30 | 23 | CB | PHE | 20 | 112.630 | 50.377 | 55.686 | 1.00 | 81.03 |
| | 24 | CG | PHE | 20 | 111.437 | 49.572 | 55.251 | 1.00 | 77.17 |
| | 25 | CD1 | PHE | 20 | 110.691 | 49.971 | 54.147 | 1.00 | 74.72 |
| | 26 | CD2 | PHE | 20 | 111.056 | 48.422 | 55.939 | 1.00 | 77.18 |
| | 27 | CE1 | PHE | 20 | 109.581 | 49.239 | 53.733 | 1.00 | 72.36 |
| 35 | 28 | CE2 | PHE | 20 | 109.947 | 47.681 | 55.535 | 1.00 | 78.10 |
| | 29 | CZ | PHE | 20 | 109.207 | 48.092 | 54.428 | 1.00 | 75.86 |
| | 30 | C | PHE | 20 | 114.280 | 50.942 | 57.465 | 1.00 | 82.49 |
| | 31 | O | PHE | 20 | 114.400 | 52.167 | 57.517 | 1.00 | 84.00 |
| | 32 | N | SER | 21 | 115.294 | 50.098 | 57.639 | 1.00 | 78.89 |
| 40 | 33 | CA | SER | 21 | 116.656 | 50.560 | 57.895 | 1.00 | 75.96 |
| | 34 | CB | SER | 21 | 117.495 | 49.433 | 58.515 | 1.00 | 75.81 |
| | 35 | OG | SER | 21 | 117.449 | 48.250 | 57.731 | 1.00 | 80.91 |
| | 36 | C | SER | 21 | 117.305 | 51.063 | 56.602 | 1.00 | 69.67 |
| | 37 | O | SER | 21 | 117.070 | 50.513 | 55.525 | 1.00 | 70.74 |
| 45 | 38 | N | PRO | 22 | 118.111 | 52.134 | 56.691 | 1.00 | 63.25 |
| | 39 | CD | PRO | 22 | 118.421 | 52.939 | 57.887 | 1.00 | 60.39 |
| | 40 | CA | PRO | 22 | 118.773 | 52.680 | 55.501 | 1.00 | 56.42 |
| | 41 | CB | PRO | 22 | 119.362 | 53.994 | 56.018 | 1.00 | 53.56 |
| | 42 | CG | PRO | 22 | 119.657 | 53.688 | 57.458 | 1.00 | 61.97 |
| 50 | 43 | C | PRO | 22 | 119.847 | 51.746 | 54.939 | 1.00 | 55.70 |

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|----|----|-----|-----|----|---------|--------|--------|------|-------|
| | 44 | O | PRO | 22 | 120.236 | 50.771 | 55.589 | 1.00 | 52.85 |
| | 45 | N | SER | 23 | 120.301 | 52.038 | 53.724 | 1.00 | 56.69 |
| | 46 | CA | SER | 23 | 121.327 | 51.233 | 53.065 | 1.00 | 53.59 |
| | 47 | CB | SER | 23 | 121.600 | 51.775 | 51.660 | 1.00 | 51.37 |
| 5 | 48 | OG | SER | 23 | 122.574 | 50.995 | 50.991 | 1.00 | 45.40 |
| | 49 | C | SER | 23 | 122.620 | 51.210 | 53.878 | 1.00 | 57.52 |
| | 50 | O | SER | 23 | 123.161 | 52.258 | 54.236 | 1.00 | 61.76 |
| | 51 | N | LEU | 24 | 123.101 | 50.004 | 54.168 | 1.00 | 58.09 |
| | 52 | CA | LEU | 24 | 124.326 | 49.799 | 54.944 | 1.00 | 55.68 |
| 10 | 53 | CB | LEU | 24 | 124.545 | 48.301 | 55.191 | 1.00 | 60.64 |
| | 54 | CG | LEU | 24 | 123.413 | 47.379 | 55.651 | 1.00 | 67.70 |
| | 55 | CD1 | LEU | 24 | 123.810 | 45.934 | 55.385 | 1.00 | 70.01 |
| | 56 | CD2 | LEU | 24 | 123.098 | 47.596 | 57.124 | 1.00 | 70.77 |
| | 57 | C | LEU | 24 | 125.554 | 50.313 | 54.198 | 1.00 | 51.07 |
| 15 | 58 | O | LEU | 24 | 126.529 | 50.754 | 54.808 | 1.00 | 50.23 |
| | 59 | N | TRP | 25 | 125.472 | 50.267 | 52.873 | 1.00 | 45.50 |
| | 60 | CA | TRP | 25 | 126.563 | 50.636 | 51.977 | 1.00 | 44.42 |
| | 61 | CB | TRP | 25 | 126.356 | 49.908 | 50.645 | 1.00 | 46.22 |
| | 62 | CG | TRP | 25 | 125.853 | 48.510 | 50.867 | 1.00 | 47.97 |
| 20 | 63 | CD2 | TRP | 25 | 126.604 | 47.407 | 51.384 | 1.00 | 50.67 |
| | 64 | CE2 | TRP | 25 | 125.700 | 46.331 | 51.553 | 1.00 | 50.91 |
| | 65 | CE3 | TRP | 25 | 127.948 | 47.219 | 51.729 | 1.00 | 45.66 |
| | 66 | CD1 | TRP | 25 | 124.567 | 48.070 | 50.732 | 1.00 | 49.99 |
| | 67 | NE1 | TRP | 25 | 124.466 | 46.765 | 51.147 | 1.00 | 47.16 |
| 25 | 68 | CZ2 | TRP | 25 | 126.101 | 45.088 | 52.053 | 1.00 | 52.99 |
| | 69 | CZ3 | TRP | 25 | 128.347 | 45.983 | 52.227 | 1.00 | 47.77 |
| | 70 | CH2 | TRP | 25 | 127.423 | 44.934 | 52.384 | 1.00 | 51.93 |
| | 71 | C | TRP | 25 | 126.893 | 52.110 | 51.744 | 1.00 | 44.49 |
| | 72 | O | TRP | 25 | 127.997 | 52.550 | 52.063 | 1.00 | 43.75 |
| 30 | 73 | N | GLY | 26 | 125.958 | 52.862 | 51.172 | 1.00 | 47.80 |
| | 74 | CA | GLY | 26 | 126.210 | 54.267 | 50.894 | 1.00 | 39.84 |
| | 75 | C | GLY | 26 | 126.744 | 54.449 | 49.483 | 1.00 | 44.69 |
| | 76 | O | GLY | 26 | 126.375 | 53.696 | 48.580 | 1.00 | 46.55 |
| | 77 | N | ASP | 27 | 127.620 | 55.434 | 49.287 | 1.00 | 46.92 |
| 35 | 78 | CA | ASP | 27 | 128.200 | 55.708 | 47.966 | 1.00 | 50.38 |
| | 79 | CB | ASP | 27 | 128.544 | 57.196 | 47.827 | 1.00 | 57.61 |
| | 80 | CG | ASP | 27 | 127.307 | 58.091 | 47.770 | 1.00 | 66.06 |
| | 81 | OD1 | ASP | 27 | 126.168 | 57.582 | 47.895 | 1.00 | 64.78 |
| | 82 | OD2 | ASP | 27 | 127.482 | 59.318 | 47.597 | 1.00 | 67.46 |
| 40 | 83 | C | ASP | 27 | 129.441 | 54.857 | 47.686 | 1.00 | 46.14 |
| | 84 | O | ASP | 27 | 130.165 | 55.082 | 46.711 | 1.00 | 47.50 |
| | 85 | N | GLN | 28 | 129.642 | 53.855 | 48.536 | 1.00 | 40.05 |
| | 86 | CA | GLN | 28 | 130.759 | 52.921 | 48.461 | 1.00 | 28.69 |
| | 87 | CB | GLN | 28 | 130.591 | 51.884 | 49.575 | 1.00 | 25.72 |
| 45 | 88 | CG | GLN | 28 | 131.624 | 50.781 | 49.615 | 1.00 | 32.15 |
| | 89 | CD | GLN | 28 | 131.331 | 49.745 | 50.688 | 1.00 | 33.15 |
| | 90 | OE1 | GLN | 28 | 131.873 | 48.643 | 50.665 | 1.00 | 41.21 |
| | 91 | NE2 | GLN | 28 | 130.467 | 50.097 | 51.638 | 1.00 | 18.55 |
| | 92 | C | GLN | 28 | 130.904 | 52.221 | 47.108 | 1.00 | 27.55 |
| 50 | 93 | O | GLN | 28 | 131.974 | 51.709 | 46.787 | 1.00 | 21.99 |

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|----|-----|-----|-----|----|---------|--------|--------|------|-------|
| | 94 | N | PHE | 29 | 129.840 | 52.223 | 46.307 | 1.00 | 27.43 |
| | 95 | CA | PHE | 29 | 129.874 | 51.561 | 45.004 | 1.00 | 26.63 |
| | 96 | CB | PHE | 29 | 128.840 | 50.432 | 44.956 | 1.00 | 33.69 |
| | 97 | CG | PHE | 29 | 129.070 | 49.349 | 45.976 | 1.00 | 28.13 |
| 5 | 98 | CD1 | PHE | 29 | 128.241 | 49.241 | 47.089 | 1.00 | 26.35 |
| | 99 | CD2 | PHE | 29 | 130.103 | 48.428 | 45.817 | 1.00 | 27.32 |
| | 100 | CE1 | PHE | 29 | 128.432 | 48.231 | 48.028 | 1.00 | 24.27 |
| | 101 | CE2 | PHE | 29 | 130.304 | 47.410 | 46.751 | 1.00 | 28.00 |
| | 102 | CZ | PHE | 29 | 129.466 | 47.311 | 47.860 | 1.00 | 16.26 |
| 10 | 103 | C | PHE | 29 | 129.712 | 52.451 | 43.771 | 1.00 | 31.14 |
| | 104 | O | PHE | 29 | 129.920 | 51.976 | 42.648 | 1.00 | 31.41 |
| | 105 | N | LEU | 30 | 129.336 | 53.718 | 43.962 | 1.00 | 33.49 |
| | 106 | CA | LEU | 30 | 129.164 | 54.658 | 42.844 | 1.00 | 39.53 |
| | 107 | CB | LEU | 30 | 128.857 | 56.065 | 43.366 | 1.00 | 47.74 |
| 15 | 108 | CG | LEU | 30 | 127.443 | 56.556 | 43.658 | 1.00 | 54.63 |
| | 109 | CD1 | LEU | 30 | 127.508 | 58.033 | 44.036 | 1.00 | 54.01 |
| | 110 | CD2 | LEU | 30 | 126.568 | 56.378 | 42.429 | 1.00 | 53.57 |
| | 111 | C | LEU | 30 | 130.433 | 54.764 | 42.009 | 1.00 | 40.75 |
| | 112 | O | LEU | 30 | 130.384 | 54.947 | 40.787 | 1.00 | 34.99 |
| 20 | 113 | N | SER | 31 | 131.565 | 54.671 | 42.696 | 1.00 | 44.10 |
| | 114 | CA | SER | 31 | 132.873 | 54.789 | 42.077 | 1.00 | 47.85 |
| | 115 | CB | SER | 31 | 133.730 | 55.737 | 42.917 | 1.00 | 53.74 |
| | 116 | OG | SER | 31 | 133.671 | 55.353 | 44.281 | 1.00 | 52.06 |
| | 117 | C | SER | 31 | 133.669 | 53.515 | 41.851 | 1.00 | 45.38 |
| 25 | 118 | O | SER | 31 | 133.909 | 52.743 | 42.782 | 1.00 | 45.28 |
| | 119 | N | PHE | 32 | 134.064 | 53.302 | 40.602 | 1.00 | 43.37 |
| | 120 | CA | PHE | 32 | 134.905 | 52.172 | 40.232 | 1.00 | 45.26 |
| | 121 | CB | PHE | 32 | 134.213 | 50.812 | 40.251 | 1.00 | 42.83 |
| | 122 | CG | PHE | 32 | 135.181 | 49.670 | 40.073 | 1.00 | 33.22 |
| 30 | 123 | CD1 | PHE | 32 | 136.098 | 49.365 | 41.075 | 1.00 | 29.45 |
| | 124 | CD2 | PHE | 32 | 135.266 | 48.984 | 38.858 | 1.00 | 32.90 |
| | 125 | CE1 | PHE | 32 | 137.096 | 48.407 | 40.875 | 1.00 | 28.42 |
| | 126 | CE2 | PHE | 32 | 136.261 | 48.023 | 38.647 | 1.00 | 27.39 |
| | 127 | CZ | PHE | 32 | 137.179 | 47.737 | 39.655 | 1.00 | 28.24 |
| 35 | 128 | C | PHE | 32 | 135.601 | 52.358 | 38.896 | 1.00 | 50.87 |
| | 129 | O | PHE | 32 | 134.988 | 52.256 | 37.829 | 1.00 | 43.81 |
| | 130 | N | SER | 33 | 136.899 | 52.626 | 38.989 | 1.00 | 55.26 |
| | 131 | CA | SER | 33 | 137.755 | 52.816 | 37.841 | 1.00 | 61.21 |
| | 132 | CB | SER | 33 | 138.587 | 54.094 | 38.017 | 1.00 | 61.87 |
| 40 | 133 | OG | SER | 33 | 139.024 | 54.250 | 39.360 | 1.00 | 67.09 |
| | 134 | C | SER | 33 | 138.641 | 51.583 | 37.731 | 1.00 | 59.75 |
| | 135 | O | SER | 33 | 139.488 | 51.329 | 38.589 | 1.00 | 59.49 |
| | 136 | N | ILE | 34 | 138.368 | 50.771 | 36.718 | 1.00 | 60.14 |
| | 137 | CA | ILE | 34 | 139.128 | 49.552 | 36.486 | 1.00 | 66.15 |
| 45 | 138 | CB | ILE | 34 | 138.426 | 48.639 | 35.442 | 1.00 | 65.50 |
| | 139 | CG2 | ILE | 34 | 138.099 | 49.423 | 34.163 | 1.00 | 69.37 |
| | 140 | CG1 | ILE | 34 | 139.291 | 47.406 | 35.157 | 1.00 | 65.37 |
| | 141 | CD1 | ILE | 34 | 138.715 | 46.458 | 34.122 | 1.00 | 63.17 |
| | 142 | C | ILE | 34 | 140.544 | 49.875 | 36.013 | 1.00 | 70.13 |
| 50 | 143 | O | ILE | 34 | 140.725 | 50.551 | 35.001 | 1.00 | 76.00 |

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|----|-----|-----|-----|----|---------|--------|--------|------|--------|
| | 144 | N | ASP | 35 | 141.545 | 49.454 | 36.782 | 1.00 | 73.05 |
| | 145 | CA | ASP | 35 | 142.935 | 49.673 | 36.388 | 1.00 | 70.88 |
| | 146 | CB | ASP | 35 | 143.895 | 49.419 | 37.558 | 1.00 | 76.13 |
| | 147 | CG | ASP | 35 | 143.288 | 48.547 | 38.638 | 1.00 | 84.32 |
| 5 | 148 | OD1 | ASP | 35 | 142.931 | 47.387 | 38.344 | 1.00 | 92.06 |
| | 149 | OD2 | ASP | 35 | 143.155 | 49.030 | 39.784 | 1.00 | 86.08 |
| | 150 | C | ASP | 35 | 143.198 | 48.714 | 35.227 | 1.00 | 68.52 |
| | 151 | O | ASP | 35 | 143.555 | 47.552 | 35.425 | 1.00 | 65.76 |
| | 152 | N | ASN | 36 | 142.940 | 49.214 | 34.019 | 1.00 | 66.53 |
| 10 | 153 | CA | ASN | 36 | 143.083 | 48.471 | 32.765 | 1.00 | 67.50 |
| | 154 | CB | ASN | 36 | 142.949 | 49.430 | 31.577 | 1.00 | 72.78 |
| | 155 | CG | ASN | 36 | 141.889 | 50.497 | 31.804 | 1.00 | 79.82 |
| | 156 | OD1 | ASN | 36 | 140.708 | 50.194 | 31.962 | 1.00 | 78.35 |
| | 157 | ND2 | ASN | 36 | 142.319 | 51.756 | 31.853 | 1.00 | 84.96 |
| 15 | 158 | C | ASN | 36 | 144.383 | 47.686 | 32.646 | 1.00 | 68.26 |
| | 159 | O | ASN | 36 | 144.461 | 46.704 | 31.906 | 1.00 | 65.02 |
| | 160 | N | GLN | 37 | 145.403 | 48.143 | 33.364 | 1.00 | 71.27 |
| | 161 | CA | GLN | 37 | 146.709 | 47.500 | 33.370 | 1.00 | 71.18 |
| | 162 | CB | GLN | 37 | 147.721 | 48.431 | 34.048 | 1.00 | 78.38 |
| 20 | 163 | CG | GLN | 37 | 149.005 | 47.761 | 34.524 | 1.00 | 90.52 |
| | 164 | CD | GLN | 37 | 149.198 | 47.904 | 36.027 | 1.00 | 100.00 |
| | 165 | OE1 | GLN | 37 | 148.538 | 48.718 | 36.673 | 1.00 | 100.00 |
| | 166 | NE2 | GLN | 37 | 150.106 | 47.105 | 36.592 | 1.00 | 100.00 |
| | 167 | C | GLN | 37 | 146.651 | 46.131 | 34.069 | 1.00 | 65.44 |
| 25 | 168 | O | GLN | 37 | 147.138 | 45.138 | 33.533 | 1.00 | 63.18 |
| | 169 | N | VAL | 38 | 146.023 | 46.086 | 35.244 | 1.00 | 57.92 |
| | 170 | CA | VAL | 38 | 145.883 | 44.849 | 36.021 | 1.00 | 51.76 |
| | 171 | CB | VAL | 38 | 145.388 | 45.152 | 37.461 | 1.00 | 50.39 |
| | 172 | CG1 | VAL | 38 | 145.198 | 43.862 | 38.251 | 1.00 | 44.02 |
| 30 | 173 | CG2 | VAL | 38 | 146.371 | 46.071 | 38.166 | 1.00 | 43.36 |
| | 174 | C | VAL | 38 | 144.916 | 43.870 | 35.349 | 1.00 | 52.33 |
| | 175 | O | VAL | 38 | 145.142 | 42.656 | 35.348 | 1.00 | 48.70 |
| | 176 | N | ALA | 39 | 143.858 | 44.412 | 34.752 | 1.00 | 49.41 |
| | 177 | CA | ALA | 39 | 142.848 | 43.610 | 34.068 | 1.00 | 48.03 |
| 35 | 178 | CB | ALA | 39 | 141.722 | 44.502 | 33.584 | 1.00 | 56.98 |
| | 179 | C | ALA | 39 | 143.434 | 42.823 | 32.900 | 1.00 | 47.68 |
| | 180 | O | ALA | 39 | 143.178 | 41.627 | 32.759 | 1.00 | 52.03 |
| | 181 | N | GLU | 40 | 144.219 | 43.501 | 32.068 | 1.00 | 46.51 |
| | 182 | CA | GLU | 40 | 144.855 | 42.881 | 30.908 | 1.00 | 40.96 |
| 40 | 183 | CB | GLU | 40 | 145.507 | 43.952 | 30.036 | 1.00 | 49.36 |
| | 184 | CG | GLU | 40 | 144.507 | 44.896 | 29.383 | 1.00 | 62.86 |
| | 185 | CD | GLU | 40 | 145.161 | 46.109 | 28.745 | 1.00 | 67.78 |
| | 186 | OE1 | GLU | 40 | 146.229 | 45.957 | 28.112 | 1.00 | 67.66 |
| | 187 | OE2 | GLU | 40 | 144.601 | 47.218 | 28.880 | 1.00 | 70.01 |
| 45 | 188 | C | GLU | 40 | 145.893 | 41.852 | 31.337 | 1.00 | 38.90 |
| | 189 | O | GLU | 40 | 146.076 | 40.832 | 30.678 | 1.00 | 39.36 |
| | 190 | N | LYS | 41 | 146.569 | 42.135 | 32.447 | 1.00 | 41.55 |
| | 191 | CA | LYS | 41 | 147.584 | 41.243 | 32.998 | 1.00 | 38.43 |
| | 192 | CB | LYS | 41 | 148.219 | 41.884 | 34.236 | 1.00 | 43.42 |
| 50 | 193 | CG | LYS | 41 | 149.304 | 41.056 | 34.903 | 1.00 | 55.00 |

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|----|-----|-----|-----|----|---------|--------|--------|------|-------|
| | 194 | CD | LYS | 41 | 149.864 | 41.780 | 36.119 | 1.00 | 61.88 |
| | 195 | CE | LYS | 41 | 151.040 | 41.028 | 36.721 | 1.00 | 62.99 |
| | 196 | NZ | LYS | 41 | 151.665 | 41.794 | 37.835 | 1.00 | 69.92 |
| | 197 | C | LYS | 41 | 146.914 | 39.926 | 33.373 | 1.00 | 36.30 |
| 5 | 198 | O | LYS | 41 | 147.362 | 38.855 | 32.966 | 1.00 | 34.80 |
| | 199 | N | TYR | 42 | 145.823 | 40.027 | 34.132 | 1.00 | 35.61 |
| | 200 | CA | TYR | 42 | 145.051 | 38.868 | 34.572 | 1.00 | 29.43 |
| | 201 | CB | TYR | 42 | 143.880 | 39.307 | 35.457 | 1.00 | 29.64 |
| | 202 | CG | TYR | 42 | 144.229 | 39.658 | 36.890 | 1.00 | 30.55 |
| 10 | 203 | CD1 | TYR | 42 | 145.556 | 39.697 | 37.330 | 1.00 | 37.21 |
| | 204 | CE1 | TYR | 42 | 145.866 | 40.002 | 38.660 | 1.00 | 37.30 |
| | 205 | CD2 | TYR | 42 | 143.222 | 39.937 | 37.814 | 1.00 | 28.62 |
| | 206 | CE2 | TYR | 42 | 143.519 | 40.241 | 39.139 | 1.00 | 37.07 |
| | 207 | CZ | TYR | 42 | 144.839 | 40.272 | 39.556 | 1.00 | 40.82 |
| 15 | 208 | OH | TYR | 42 | 145.121 | 40.567 | 40.869 | 1.00 | 43.81 |
| | 209 | C | TYR | 42 | 144.499 | 38.097 | 33.377 | 1.00 | 30.40 |
| | 210 | O | TYR | 42 | 144.603 | 36.872 | 33.318 | 1.00 | 29.10 |
| | 211 | N | ALA | 43 | 143.920 | 38.827 | 32.426 | 1.00 | 24.33 |
| | 212 | CA | ALA | 43 | 143.340 | 38.227 | 31.227 | 1.00 | 29.09 |
| 20 | 213 | CB | ALA | 43 | 142.713 | 39.308 | 30.356 | 1.00 | 19.04 |
| | 214 | C | ALA | 43 | 144.358 | 37.423 | 30.421 | 1.00 | 29.23 |
| | 215 | O | ALA | 43 | 144.074 | 36.308 | 29.984 | 1.00 | 29.14 |
| | 216 | N | LYS | 44 | 145.559 | 37.972 | 30.260 | 1.00 | 37.81 |
| | 217 | CA | LYS | 44 | 146.637 | 37.371 | 29.491 | 1.00 | 40.64 |
| 25 | 218 | C | LYS | 44 | 147.069 | 36.041 | 30.095 | 1.00 | 34.80 |
| | 219 | O | LYS | 44 | 147.221 | 35.048 | 29.357 | 1.00 | 35.25 |
| | 220 | CB | LYS | 44 | 147.824 | 38.329 | 29.396 | 1.00 | 54.18 |
| | 221 | CG | LYS | 44 | 149.001 | 37.784 | 28.605 | 1.00 | 67.03 |
| | 222 | CD | LYS | 44 | 150.141 | 38.787 | 28.552 | 1.00 | 79.04 |
| 30 | 223 | CE | LYS | 44 | 151.313 | 38.247 | 27.750 | 1.00 | 20.00 |
| | 224 | NZ | LYS | 44 | 152.431 | 39.227 | 27.673 | 1.00 | 20.00 |
| | 225 | N | GLU | 45 | 147.332 | 36.000 | 31.397 | 1.00 | 31.47 |
| | 226 | CA | GLU | 45 | 147.771 | 34.779 | 32.070 | 1.00 | 30.36 |
| | 227 | CB | GLU | 45 | 148.288 | 35.080 | 33.480 | 1.00 | 26.58 |
| 35 | 228 | CG | GLU | 45 | 149.071 | 33.920 | 34.105 | 1.00 | 19.97 |
| | 229 | CD | GLU | 45 | 149.394 | 34.128 | 35.580 | 1.00 | 33.35 |
| | 230 | OE1 | GLU | 45 | 149.791 | 33.146 | 36.246 | 1.00 | 31.26 |
| | 231 | OE2 | GLU | 45 | 149.249 | 35.264 | 36.080 | 1.00 | 37.21 |
| | 232 | C | GLU | 45 | 146.649 | 33.747 | 32.142 | 1.00 | 31.64 |
| 40 | 233 | O | GLU | 45 | 146.902 | 32.545 | 32.058 | 1.00 | 38.67 |
| | 234 | N | ILE | 46 | 145.415 | 34.225 | 32.299 | 1.00 | 34.27 |
| | 235 | CA | ILE | 46 | 144.239 | 33.358 | 32.373 | 1.00 | 30.12 |
| | 236 | CB | ILE | 46 | 142.942 | 34.181 | 32.608 | 1.00 | 33.74 |
| | 237 | CG2 | ILE | 46 | 141.706 | 33.420 | 32.123 | 1.00 | 32.63 |
| 45 | 238 | CG1 | ILE | 46 | 142.812 | 34.534 | 34.093 | 1.00 | 34.26 |
| | 239 | CD1 | ILE | 46 | 141.644 | 35.444 | 34.407 | 1.00 | 30.01 |
| | 240 | C | ILE | 46 | 144.099 | 32.518 | 31.110 | 1.00 | 29.77 |
| | 241 | O | ILE | 46 | 143.850 | 31.315 | 31.186 | 1.00 | 30.24 |
| | 242 | N | GLU | 47 | 144.283 | 33.156 | 29.956 | 1.00 | 31.42 |
| 50 | 243 | CA | GLU | 47 | 144.185 | 32.482 | 28.666 | 1.00 | 37.34 |

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|----|-----|-----|-----|----|---------|--------|--------|------|-------|
| | 244 | CB | GLU | 47 | 144.460 | 33.476 | 27.537 | 1.00 | 45.72 |
| | 245 | CG | GLU | 47 | 144.290 | 32.896 | 26.137 | 1.00 | 68.61 |
| | 246 | CD | GLU | 47 | 144.808 | 33.813 | 25.035 | 1.00 | 79.62 |
| | 247 | OE1 | GLU | 47 | 145.302 | 34.922 | 25.339 | 1.00 | 89.55 |
| 5 | 248 | OE2 | GLU | 47 | 144.728 | 33.417 | 23.852 | 1.00 | 86.41 |
| | 249 | C | GLU | 47 | 145.169 | 31.314 | 28.580 | 1.00 | 37.12 |
| | 250 | O | GLU | 47 | 144.860 | 30.275 | 27.997 | 1.00 | 45.60 |
| | 251 | N | ALA | 48 | 146.348 | 31.492 | 29.171 | 1.00 | 33.83 |
| | 252 | CA | ALA | 48 | 147.378 | 30.459 | 29.170 | 1.00 | 30.76 |
| 10 | 253 | CB | ALA | 48 | 148.720 | 31.054 | 29.575 | 1.00 | 33.78 |
| | 254 | C | ALA | 48 | 146.986 | 29.323 | 30.110 | 1.00 | 30.08 |
| | 255 | O | ALA | 48 | 147.071 | 28.150 | 29.743 | 1.00 | 30.80 |
| | 256 | N | LEU | 49 | 146.542 | 29.685 | 31.312 | 1.00 | 27.01 |
| | 257 | CA | LEU | 49 | 146.110 | 28.720 | 32.321 | 1.00 | 23.68 |
| 15 | 258 | CB | LEU | 49 | 145.793 | 29.445 | 33.628 | 1.00 | 19.74 |
| | 259 | CG | LEU | 49 | 146.936 | 30.167 | 34.337 | 1.00 | 15.12 |
| | 260 | CD1 | LEU | 49 | 146.368 | 31.161 | 35.328 | 1.00 | 8.67 |
| | 261 | CD2 | LEU | 49 | 147.844 | 29.164 | 35.033 | 1.00 | 12.64 |
| | 262 | C | LEU | 49 | 144.862 | 27.985 | 31.836 | 1.00 | 24.27 |
| 20 | 263 | O | LEU | 49 | 144.610 | 26.842 | 32.214 | 1.00 | 31.26 |
| | 264 | N | LYS | 50 | 144.101 | 28.663 | 30.983 | 1.00 | 27.77 |
| | 265 | CA | LYS | 50 | 142.863 | 28.154 | 30.394 | 1.00 | 30.88 |
| | 266 | CB | LYS | 50 | 142.247 | 29.263 | 29.548 | 1.00 | 31.45 |
| | 267 | CG | LYS | 50 | 140.775 | 29.153 | 29.242 | 1.00 | 31.65 |
| 25 | 268 | CD | LYS | 50 | 140.333 | 30.468 | 28.621 | 1.00 | 33.98 |
| | 269 | CE | LYS | 50 | 138.871 | 30.468 | 28.250 | 1.00 | 42.53 |
| | 270 | NZ | LYS | 50 | 138.455 | 31.817 | 27.773 | 1.00 | 47.24 |
| | 271 | C | LYS | 50 | 143.120 | 26.925 | 29.527 | 1.00 | 32.84 |
| | 272 | O | LYS | 50 | 142.449 | 25.901 | 29.675 | 1.00 | 31.46 |
| 30 | 273 | N | GLU | 51 | 144.092 | 27.033 | 28.625 | 1.00 | 33.57 |
| | 274 | CA | GLU | 51 | 144.439 | 25.927 | 27.741 | 1.00 | 38.44 |
| | 275 | CB | GLU | 51 | 145.286 | 26.416 | 26.566 | 1.00 | 45.31 |
| | 276 | CG | GLU | 51 | 145.241 | 25.501 | 25.339 | 1.00 | 54.99 |
| | 277 | CD | GLU | 51 | 143.953 | 25.633 | 24.532 | 1.00 | 61.58 |
| 35 | 278 | OE1 | GLU | 51 | 143.086 | 26.463 | 24.893 | 1.00 | 63.41 |
| | 279 | OE2 | GLU | 51 | 143.815 | 24.912 | 23.519 | 1.00 | 63.99 |
| | 280 | C | GLU | 51 | 145.179 | 24.824 | 28.501 | 1.00 | 37.86 |
| | 281 | O | GLU | 51 | 145.145 | 23.662 | 28.097 | 1.00 | 43.06 |
| | 282 | N | GLN | 52 | 145.867 | 25.192 | 29.582 | 1.00 | 36.20 |
| 40 | 283 | CA | GLN | 52 | 146.592 | 24.212 | 30.397 | 1.00 | 38.10 |
| | 284 | CB | GLN | 52 | 147.453 | 24.897 | 31.465 | 1.00 | 41.72 |
| | 285 | CG | GLN | 52 | 148.691 | 25.615 | 30.943 | 1.00 | 47.34 |
| | 286 | CD | GLN | 52 | 149.505 | 26.249 | 32.061 | 1.00 | 49.46 |
| | 287 | OE1 | GLN | 52 | 149.640 | 25.683 | 33.145 | 1.00 | 43.98 |
| 45 | 288 | NE2 | GLN | 52 | 150.049 | 27.438 | 31.799 | 1.00 | 53.90 |
| | 289 | C | GLN | 52 | 145.563 | 23.339 | 31.093 | 1.00 | 38.87 |
| | 290 | O | GLN | 52 | 145.732 | 22.122 | 31.219 | 1.00 | 40.47 |
| | 291 | N | THR | 53 | 144.501 | 23.991 | 31.554 | 1.00 | 37.87 |
| | 292 | CA | THR | 53 | 143.407 | 23.323 | 32.236 | 1.00 | 32.77 |
| 50 | 293 | CB | THR | 53 | 142.541 | 24.347 | 32.992 | 1.00 | 31.08 |

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|----|-----|-----|-----|----|---------|--------|--------|------|-------|
| | 294 | OG1 | THR | 53 | 143.315 | 24.933 | 34.050 | 1.00 | 28.04 |
| | 295 | CG2 | THR | 53 | 141.296 | 23.685 | 33.569 | 1.00 | 32.90 |
| | 296 | C | THR | 53 | 142.570 | 22.522 | 31.233 | 1.00 | 32.05 |
| 5 | 297 | O | THR | 53 | 142.013 | 21.476 | 31.573 | 1.00 | 29.73 |
| | 298 | N | ARG | 54 | 142.529 | 22.992 | 29.988 | 1.00 | 28.01 |
| | 299 | CA | ARG | 54 | 141.785 | 22.312 | 28.933 | 1.00 | 23.69 |
| | 300 | CB | ARG | 54 | 141.723 | 23.176 | 27.673 | 1.00 | 23.31 |
| | 301 | CG | ARG | 54 | 140.724 | 22.682 | 26.633 | 1.00 | 24.23 |
| 10 | 302 | CD | ARG | 54 | 140.755 | 23.527 | 25.360 | 1.00 | 30.78 |
| | 303 | NE | ARG | 54 | 140.674 | 24.969 | 25.619 | 1.00 | 45.26 |
| | 304 | CZ | ARG | 54 | 139.564 | 25.633 | 25.942 | 1.00 | 46.57 |
| | 305 | NH1 | ARG | 54 | 138.405 | 24.999 | 26.058 | 1.00 | 51.75 |
| | 306 | NH2 | ARG | 54 | 139.608 | 26.946 | 26.140 | 1.00 | 43.00 |
| | 307 | C | ARG | 54 | 142.487 | 20.998 | 28.617 | 1.00 | 30.27 |
| 15 | 308 | O | ARG | 54 | 141.842 | 19.955 | 28.479 | 1.00 | 33.41 |
| | 309 | N | ASN | 55 | 143.821 | 21.050 | 28.526 | 1.00 | 33.72 |
| | 310 | CA | ASN | 55 | 144.648 | 19.899 | 28.240 | 1.00 | 33.22 |
| | 311 | C | ASN | 55 | 144.538 | 18.872 | 29.348 | 1.00 | 35.28 |
| 20 | 312 | O | ASN | 55 | 144.679 | 17.660 | 29.105 | 1.00 | 35.19 |
| | 313 | CB | ASN | 55 | 146.080 | 20.341 | 27.963 | 1.00 | 36.29 |
| | 314 | CG | ASN | 55 | 146.150 | 21.264 | 26.761 | 1.00 | 20.00 |
| | 315 | OD1 | ASN | 55 | 145.473 | 21.038 | 25.754 | 1.00 | 20.00 |
| | 316 | ND2 | ASN | 55 | 146.963 | 22.307 | 26.857 | 1.00 | 20.00 |
| | 317 | N | MET | 56 | 144.309 | 19.330 | 30.581 | 1.00 | 34.89 |
| 25 | 318 | CA | MET | 56 | 144.150 | 18.442 | 31.734 | 1.00 | 34.60 |
| | 319 | CB | MET | 56 | 144.058 | 19.241 | 33.039 | 1.00 | 27.26 |
| | 320 | CG | MET | 56 | 145.378 | 19.792 | 33.544 | 1.00 | 38.81 |
| | 321 | SD | MET | 56 | 145.237 | 20.594 | 35.159 | 1.00 | 40.35 |
| | 322 | CE | MET | 56 | 145.790 | 22.242 | 34.734 | 1.00 | 41.02 |
| 30 | 323 | C | MET | 56 | 142.880 | 17.606 | 31.560 | 1.00 | 38.38 |
| | 324 | O | MET | 56 | 142.871 | 16.406 | 31.847 | 1.00 | 36.10 |
| | 325 | N | LEU | 57 | 141.816 | 18.253 | 31.084 | 1.00 | 33.14 |
| | 326 | CA | LEU | 57 | 140.535 | 17.593 | 30.852 | 1.00 | 33.61 |
| | 327 | CB | LEU | 57 | 139.444 | 18.633 | 30.566 | 1.00 | 24.13 |
| 35 | 328 | CG | LEU | 57 | 138.939 | 19.472 | 31.742 | 1.00 | 25.14 |
| | 329 | CD1 | LEU | 57 | 138.092 | 20.624 | 31.235 | 1.00 | 18.69 |
| | 330 | CD2 | LEU | 57 | 138.143 | 18.604 | 32.703 | 1.00 | 10.16 |
| | 331 | C | LEU | 57 | 140.610 | 16.611 | 29.686 | 1.00 | 37.09 |
| | 332 | O | LEU | 57 | 139.922 | 15.588 | 29.679 | 1.00 | 34.95 |
| 40 | 333 | N | LEU | 58 | 141.453 | 16.924 | 28.703 | 1.00 | 35.34 |
| | 334 | CA | LEU | 58 | 141.605 | 16.071 | 27.533 | 1.00 | 35.75 |
| | 335 | CB | LEU | 58 | 141.930 | 16.926 | 26.304 | 1.00 | 33.37 |
| | 336 | CG | LEU | 58 | 140.886 | 17.987 | 25.951 | 1.00 | 36.57 |
| | 337 | CD1 | LEU | 58 | 141.334 | 18.779 | 24.736 | 1.00 | 34.54 |
| 45 | 338 | CD2 | LEU | 58 | 139.540 | 17.333 | 25.691 | 1.00 | 38.57 |
| | 339 | C | LEU | 58 | 142.628 | 14.946 | 27.688 | 1.00 | 40.17 |
| | 340 | O | LEU | 58 | 143.001 | 14.298 | 26.710 | 1.00 | 38.69 |
| | 341 | N | ALA | 59 | 143.066 | 14.697 | 28.922 | 1.00 | 45.53 |
| | 342 | CA | ALA | 59 | 144.038 | 13.637 | 29.198 | 1.00 | 52.73 |
| 50 | 343 | CB | ALA | 59 | 144.562 | 13.754 | 30.626 | 1.00 | 52.29 |

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|----|-----|-----|-----|----|---------|--------|--------|------|-------|
| | 344 | C | ALA | 59 | 143.402 | 12.263 | 28.950 | 1.00 | 60.58 |
| | 345 | O | ALA | 59 | 142.320 | 11.962 | 29.450 | 1.00 | 62.17 |
| | 346 | N | THR | 60 | 144.084 | 11.432 | 28.168 | 1.00 | 63.55 |
| 5 | 347 | CA | THR | 60 | 143.575 | 10.109 | 27.794 | 1.00 | 63.50 |
| | 348 | CB | THR | 60 | 144.405 | 9.528 | 26.641 | 1.00 | 63.61 |
| | 349 | OG1 | THR | 60 | 145.776 | 9.434 | 27.039 | 1.00 | 67.85 |
| | 350 | CG2 | THR | 60 | 144.302 | 10.426 | 25.420 | 1.00 | 59.57 |
| | 351 | C | THR | 60 | 143.372 | 9.004 | 28.844 | 1.00 | 64.51 |
| 10 | 352 | O | THR | 60 | 142.237 | 8.681 | 29.198 | 1.00 | 69.94 |
| | 353 | N | GLY | 61 | 144.470 | 8.435 | 29.337 | 1.00 | 59.72 |
| | 354 | CA | GLY | 61 | 144.394 | 7.339 | 30.294 | 1.00 | 59.70 |
| | 355 | C | GLY | 61 | 144.087 | 7.572 | 31.767 | 1.00 | 60.15 |
| | 356 | O | GLY | 61 | 144.627 | 6.862 | 32.620 | 1.00 | 62.75 |
| 15 | 357 | N | MET | 62 | 143.233 | 8.546 | 32.098 | 1.00 | 62.09 |
| | 358 | CA | MET | 62 | 142.904 | 8.860 | 33.482 | 1.00 | 62.20 |
| | 359 | C | MET | 62 | 141.787 | 7.962 | 34.001 | 1.00 | 57.87 |
| | 360 | O | MET | 62 | 140.858 | 7.592 | 33.304 | 1.00 | 60.93 |
| | 361 | CB | MET | 62 | 142.512 | 10.333 | 33.619 | 1.00 | 65.78 |
| 20 | 362 | CG | MET | 62 | 142.374 | 10.806 | 35.057 | 1.00 | 71.62 |
| | 363 | SD | MET | 62 | 141.924 | 12.547 | 35.177 | 1.00 | 20.00 |
| | 364 | CE | MET | 62 | 141.630 | 12.940 | 33.455 | 1.00 | 20.00 |
| | 365 | N | LYS | 63 | 141.877 | 7.621 | 35.308 | 1.00 | 53.67 |
| | 366 | CA | LYS | 63 | 140.886 | 6.787 | 35.975 | 1.00 | 51.44 |
| 25 | 367 | CB | LYS | 63 | 141.401 | 6.323 | 37.342 | 1.00 | 55.26 |
| | 368 | CG | LYS | 63 | 142.607 | 5.402 | 37.287 | 1.00 | 65.11 |
| | 369 | CD | LYS | 63 | 142.968 | 4.915 | 38.682 | 1.00 | 69.24 |
| | 370 | CE | LYS | 63 | 144.127 | 3.936 | 38.635 | 1.00 | 76.58 |
| | 371 | NZ | LYS | 63 | 144.434 | 3.376 | 39.980 | 1.00 | 78.96 |
| 30 | 372 | C | LYS | 63 | 139.576 | 7.543 | 36.173 | 1.00 | 48.71 |
| | 373 | O | LYS | 63 | 139.559 | 8.778 | 36.167 | 1.00 | 48.30 |
| | 374 | N | LEU | 64 | 138.490 | 6.802 | 36.386 | 1.00 | 44.07 |
| | 375 | CA | LEU | 64 | 137.182 | 7.413 | 36.586 | 1.00 | 38.53 |
| | 376 | CB | LEU | 64 | 136.100 | 6.343 | 36.778 | 1.00 | 40.14 |
| 35 | 377 | CG | LEU | 64 | 134.671 | 6.886 | 36.899 | 1.00 | 35.60 |
| | 378 | CD1 | LEU | 64 | 134.283 | 7.589 | 35.606 | 1.00 | 32.53 |
| | 379 | CD2 | LEU | 64 | 133.689 | 5.773 | 37.203 | 1.00 | 30.12 |
| | 380 | C | LEU | 64 | 137.184 | 8.363 | 37.778 | 1.00 | 32.66 |
| | 381 | O | LEU | 64 | 136.773 | 9.515 | 37.650 | 1.00 | 32.91 |
| 40 | 382 | N | ALA | 65 | 137.664 | 7.881 | 38.923 | 1.00 | 26.30 |
| | 383 | CA | ALA | 65 | 137.721 | 8.683 | 40.141 | 1.00 | 27.29 |
| | 384 | CB | ALA | 65 | 138.362 | 7.885 | 41.265 | 1.00 | 26.12 |
| | 385 | C | ALA | 65 | 138.482 | 9.988 | 39.919 | 1.00 | 33.96 |
| | 386 | O | ALA | 65 | 138.019 | 11.057 | 40.318 | 1.00 | 35.01 |
| 45 | 387 | N | ASP | 66 | 139.630 | 9.897 | 39.250 | 1.00 | 35.46 |
| | 388 | CA | ASP | 66 | 140.459 | 11.064 | 38.961 | 1.00 | 35.10 |
| | 389 | CB | ASP | 66 | 141.776 | 10.646 | 38.298 | 1.00 | 36.60 |
| | 390 | CG | ASP | 66 | 142.685 | 9.867 | 39.229 | 1.00 | 34.65 |
| | 391 | OD1 | ASP | 66 | 142.611 | 10.067 | 40.461 | 1.00 | 25.86 |
| | 392 | OD2 | ASP | 66 | 143.488 | 9.057 | 38.717 | 1.00 | 44.77 |
| 50 | 393 | C | ASP | 66 | 139.746 | 12.065 | 38.059 | 1.00 | 31.14 |

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|----|-----|-----|-----|----|---------|--------|--------|------|-------|
| | 394 | O | ASP | 66 | 139.846 | 13.276 | 38.266 | 1.00 | 31.51 |
| | 395 | N | THR | 67 | 139.045 | 11.552 | 37.051 | 1.00 | 26.69 |
| | 396 | CA | THR | 67 | 138.316 | 12.392 | 36.105 | 1.00 | 26.40 |
| | 397 | CB | THR | 67 | 137.793 | 11.571 | 34.918 | 1.00 | 25.70 |
| 5 | 398 | OG1 | THR | 67 | 138.891 | 10.917 | 34.270 | 1.00 | 27.33 |
| | 399 | CG2 | THR | 67 | 137.095 | 12.474 | 33.918 | 1.00 | 28.90 |
| | 400 | C | THR | 67 | 137.146 | 13.113 | 36.769 | 1.00 | 24.73 |
| | 401 | O | THR | 67 | 136.899 | 14.290 | 36.502 | 1.00 | 27.41 |
| | 402 | N | LEU | 68 | 136.425 | 12.401 | 37.629 | 1.00 | 23.13 |
| 10 | 403 | CA | LEU | 68 | 135.295 | 12.985 | 38.333 | 1.00 | 18.00 |
| | 404 | CB | LEU | 68 | 134.504 | 11.909 | 39.078 | 1.00 | 13.23 |
| | 405 | CG | LEU | 68 | 133.804 | 10.871 | 38.201 | 1.00 | 16.24 |
| | 406 | CD1 | LEU | 68 | 133.109 | 9.843 | 39.078 | 1.00 | 17.55 |
| | 407 | CD2 | LEU | 68 | 132.811 | 11.552 | 37.272 | 1.00 | 7.96 |
| 15 | 408 | C | LEU | 68 | 135.787 | 14.047 | 39.305 | 1.00 | 19.40 |
| | 409 | O | LEU | 68 | 135.181 | 15.113 | 39.420 | 1.00 | 21.96 |
| | 410 | N | ASN | 69 | 136.899 | 13.766 | 39.980 | 1.00 | 17.72 |
| | 411 | CA | ASN | 69 | 137.471 | 14.714 | 40.931 | 1.00 | 23.29 |
| | 412 | CB | ASN | 69 | 138.608 | 14.071 | 41.728 | 1.00 | 27.45 |
| 20 | 413 | CG | ASN | 69 | 138.102 | 13.102 | 42.783 | 1.00 | 44.15 |
| | 414 | OD1 | ASN | 69 | 137.171 | 13.413 | 43.530 | 1.00 | 45.05 |
| | 415 | ND2 | ASN | 69 | 138.709 | 11.921 | 42.846 | 1.00 | 48.60 |
| | 416 | C | ASN | 69 | 137.954 | 15.985 | 40.240 | 1.00 | 21.73 |
| | 417 | O | ASN | 69 | 137.784 | 17.083 | 40.764 | 1.00 | 19.56 |
| 25 | 418 | N | LEU | 70 | 138.526 | 15.834 | 39.050 | 1.00 | 19.22 |
| | 419 | CA | LEU | 70 | 139.012 | 16.979 | 38.293 | 1.00 | 18.06 |
| | 420 | CB | LEU | 70 | 139.736 | 16.522 | 37.025 | 1.00 | 14.83 |
| | 421 | CG | LEU | 70 | 140.274 | 17.650 | 36.141 | 1.00 | 18.22 |
| | 422 | CD1 | LEU | 70 | 141.330 | 18.446 | 36.889 | 1.00 | 15.05 |
| 30 | 423 | CD2 | LEU | 70 | 140.845 | 17.078 | 34.862 | 1.00 | 20.94 |
| | 424 | C | LEU | 70 | 137.835 | 17.871 | 37.925 | 1.00 | 20.53 |
| | 425 | O | LEU | 70 | 137.844 | 19.069 | 38.212 | 1.00 | 23.73 |
| | 426 | N | ILE | 71 | 136.817 | 17.269 | 37.312 | 1.00 | 19.75 |
| | 427 | CA | ILE | 71 | 135.613 | 17.986 | 36.901 | 1.00 | 16.33 |
| 35 | 428 | CB | ILE | 71 | 134.617 | 17.043 | 36.184 | 1.00 | 19.20 |
| | 429 | CG2 | ILE | 71 | 133.278 | 17.744 | 35.950 | 1.00 | 17.41 |
| | 430 | CG1 | ILE | 71 | 135.216 | 16.574 | 34.856 | 1.00 | 25.29 |
| | 431 | CD1 | ILE | 71 | 134.273 | 15.748 | 34.009 | 1.00 | 21.71 |
| | 432 | C | ILE | 71 | 134.927 | 18.661 | 38.088 | 1.00 | 15.45 |
| 40 | 433 | O | ILE | 71 | 134.507 | 19.813 | 37.991 | 1.00 | 10.60 |
| | 434 | N | ASP | 72 | 134.846 | 17.952 | 39.212 | 1.00 | 14.16 |
| | 435 | CA | ASP | 72 | 134.222 | 18.477 | 40.425 | 1.00 | 13.13 |
| | 436 | CB | ASP | 72 | 134.206 | 17.400 | 41.516 | 1.00 | 9.28 |
| | 437 | CG | ASP | 72 | 133.456 | 17.828 | 42.766 | 1.00 | 8.19 |
| 45 | 438 | OD1 | ASP | 72 | 132.472 | 18.591 | 42.660 | 1.00 | 19.56 |
| | 439 | OD2 | ASP | 72 | 133.842 | 17.381 | 43.865 | 1.00 | 24.87 |
| | 440 | C | ASP | 72 | 134.969 | 19.709 | 40.926 | 1.00 | 20.93 |
| | 441 | O | ASP | 72 | 134.357 | 20.734 | 41.230 | 1.00 | 31.87 |
| | 442 | N | THR | 73 | 136.298 | 19.618 | 40.980 | 1.00 | 26.21 |
| 50 | 443 | CA | THR | 73 | 137.162 | 20.689 | 41.452 | 1.00 | 17.72 |

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|----|-----|-----|-----|----|---------|--------|--------|------|-------|
| | 444 | C | THR | 73 | 137.051 | 21.912 | 40.558 | 1.00 | 16.99 |
| | 445 | O | THR | 73 | 136.913 | 23.046 | 41.054 | 1.00 | 15.04 |
| | 446 | CB | THR | 73 | 138.627 | 20.258 | 41.508 | 1.00 | 18.68 |
| | 447 | OG1 | THR | 73 | 138.771 | 19.152 | 42.406 | 1.00 | 20.00 |
| 5 | 448 | CG2 | THR | 73 | 139.503 | 21.413 | 41.971 | 1.00 | 23.27 |
| | 449 | N | ILE | 74 | 137.124 | 21.732 | 39.245 | 1.00 | 13.35 |
| | 450 | CA | ILE | 74 | 137.024 | 22.837 | 38.298 | 1.00 | 15.24 |
| | 451 | CB | ILE | 74 | 137.214 | 22.342 | 36.844 | 1.00 | 17.48 |
| | 452 | CG2 | ILE | 74 | 136.841 | 23.434 | 35.843 | 1.00 | 10.21 |
| 10 | 453 | CG1 | ILE | 74 | 138.658 | 21.881 | 36.637 | 1.00 | 16.00 |
| | 454 | CD1 | ILE | 74 | 138.936 | 21.335 | 35.253 | 1.00 | 19.68 |
| | 455 | C | ILE | 74 | 135.677 | 23.554 | 38.431 | 1.00 | 21.97 |
| | 456 | O | ILE | 74 | 135.603 | 24.774 | 38.285 | 1.00 | 37.27 |
| | 457 | N | GLU | 75 | 134.620 | 22.793 | 38.712 | 1.00 | 24.94 |
| 15 | 458 | CA | GLU | 75 | 133.283 | 23.362 | 38.869 | 1.00 | 17.86 |
| | 459 | CB | GLU | 75 | 132.216 | 22.266 | 38.893 | 1.00 | 22.45 |
| | 460 | CG | GLU | 75 | 131.998 | 21.565 | 37.557 | 1.00 | 23.19 |
| | 461 | CD | GLU | 75 | 130.753 | 20.685 | 37.539 | 1.00 | 24.24 |
| | 462 | OE1 | GLU | 75 | 130.485 | 19.984 | 38.540 | 1.00 | 11.68 |
| 20 | 463 | OE2 | GLU | 75 | 130.041 | 20.699 | 36.513 | 1.00 | 19.29 |
| | 464 | C | GLU | 75 | 133.194 | 24.181 | 40.142 | 1.00 | 16.49 |
| | 465 | O | GLU | 75 | 132.739 | 25.323 | 40.119 | 1.00 | 18.93 |
| | 466 | N | ARG | 76 | 133.640 | 23.590 | 41.248 | 1.00 | 11.73 |
| | 467 | CA | ARG | 76 | 133.626 | 24.248 | 42.552 | 1.00 | 15.45 |
| 25 | 468 | CB | ARG | 76 | 134.114 | 23.282 | 43.636 | 1.00 | 7.10 |
| | 469 | CG | ARG | 76 | 133.198 | 22.097 | 43.899 | 1.00 | 15.61 |
| | 470 | CD | ARG | 76 | 133.785 | 21.197 | 44.975 | 1.00 | 12.16 |
| | 471 | NE | ARG | 76 | 132.824 | 20.231 | 45.508 | 1.00 | 16.00 |
| | 472 | CZ | ARG | 76 | 132.467 | 20.165 | 46.789 | 1.00 | 19.23 |
| 30 | 473 | NH1 | ARG | 76 | 132.982 | 21.010 | 47.670 | 1.00 | 26.80 |
| | 474 | NH2 | ARG | 76 | 131.618 | 19.234 | 47.202 | 1.00 | 29.06 |
| | 475 | C | ARG | 76 | 134.486 | 25.519 | 42.564 | 1.00 | 20.45 |
| | 476 | O | ARG | 76 | 134.214 | 26.454 | 43.319 | 1.00 | 19.47 |
| | 477 | N | LEU | 77 | 135.525 | 25.539 | 41.732 | 1.00 | 20.12 |
| 35 | 478 | CA | LEU | 77 | 136.419 | 26.692 | 41.634 | 1.00 | 19.40 |
| | 479 | CB | LEU | 77 | 137.756 | 26.281 | 41.014 | 1.00 | 12.91 |
| | 480 | CG | LEU | 77 | 138.678 | 25.382 | 41.843 | 1.00 | 12.12 |
| | 481 | CD1 | LEU | 77 | 139.825 | 24.903 | 40.973 | 1.00 | 2.00 |
| | 482 | CD2 | LEU | 77 | 139.201 | 26.125 | 43.070 | 1.00 | 4.07 |
| 40 | 483 | C | LEU | 77 | 135.796 | 27.823 | 40.818 | 1.00 | 22.31 |
| | 484 | O | LEU | 77 | 136.374 | 28.906 | 40.702 | 1.00 | 30.09 |
| | 485 | N | GLY | 78 | 134.628 | 27.551 | 40.238 | 1.00 | 26.16 |
| | 486 | CA | GLY | 78 | 133.915 | 28.542 | 39.447 | 1.00 | 20.26 |
| | 487 | C | GLY | 78 | 134.496 | 28.855 | 38.082 | 1.00 | 16.66 |
| 45 | 488 | O | GLY | 78 | 134.185 | 29.898 | 37.504 | 1.00 | 19.22 |
| | 489 | N | ILE | 79 | 135.323 | 27.959 | 37.553 | 1.00 | 13.23 |
| | 490 | CA | ILE | 79 | 135.938 | 28.179 | 36.247 | 1.00 | 16.00 |
| | 491 | CB | ILE | 79 | 137.488 | 28.083 | 36.321 | 1.00 | 14.32 |
| | 492 | CG2 | ILE | 79 | 138.055 | 29.257 | 37.111 | 1.00 | 9.65 |
| 50 | 493 | CG1 | ILE | 79 | 137.909 | 26.751 | 36.944 | 1.00 | 15.84 |

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|----|-----|-----|-----|----|---------|--------|--------|------|-------|
| | 494 | CD1 | ILE | 79 | 139.413 | 26.574 | 37.082 | 1.00 | 20.69 |
| | 495 | C | ILE | 79 | 135.420 | 27.216 | 35.185 | 1.00 | 17.13 |
| | 496 | O | ILE | 79 | 135.860 | 27.256 | 34.033 | 1.00 | 20.55 |
| | 497 | N | SER | 80 | 134.459 | 26.377 | 35.567 | 1.00 | 21.41 |
| 5 | 498 | CA | SER | 80 | 133.878 | 25.392 | 34.654 | 1.00 | 23.76 |
| | 499 | CB | SER | 80 | 133.004 | 24.393 | 35.419 | 1.00 | 20.88 |
| | 500 | OG | SER | 80 | 131.996 | 25.047 | 36.170 | 1.00 | 23.54 |
| | 501 | C | SER | 80 | 133.093 | 25.977 | 33.485 | 1.00 | 20.44 |
| | 502 | O | SER | 80 | 132.839 | 25.280 | 32.505 | 1.00 | 28.56 |
| 10 | 503 | N | TYR | 81 | 132.723 | 27.252 | 33.577 | 1.00 | 18.39 |
| | 504 | CA | TYR | 81 | 131.972 | 27.907 | 32.507 | 1.00 | 19.66 |
| | 505 | CB | TYR | 81 | 131.389 | 29.244 | 32.986 | 1.00 | 10.58 |
| | 506 | CG | TYR | 81 | 132.396 | 30.362 | 33.170 | 1.00 | 19.55 |
| | 507 | CD1 | TYR | 81 | 132.635 | 31.285 | 32.151 | 1.00 | 26.56 |
| 15 | 508 | CE1 | TYR | 81 | 133.540 | 32.331 | 32.320 | 1.00 | 23.18 |
| | 509 | CD2 | TYR | 81 | 133.092 | 30.513 | 34.367 | 1.00 | 12.72 |
| | 510 | CE2 | TYR | 81 | 133.998 | 31.555 | 34.546 | 1.00 | 18.75 |
| | 511 | CZ | TYR | 81 | 134.218 | 32.460 | 33.519 | 1.00 | 21.59 |
| | 512 | OH | TYR | 81 | 135.122 | 33.487 | 33.688 | 1.00 | 23.90 |
| 20 | 513 | C | TYR | 81 | 132.814 | 28.103 | 31.240 | 1.00 | 23.33 |
| | 514 | O | TYR | 81 | 132.294 | 28.498 | 30.195 | 1.00 | 26.36 |
| | 515 | N | HIS | 82 | 134.114 | 27.835 | 31.352 | 1.00 | 27.33 |
| | 516 | CA | HIS | 82 | 135.044 | 27.955 | 30.229 | 1.00 | 28.77 |
| | 517 | CB | HIS | 82 | 136.471 | 28.227 | 30.724 | 1.00 | 20.70 |
| 25 | 518 | CG | HIS | 82 | 136.676 | 29.592 | 31.301 | 1.00 | 18.33 |
| | 519 | CD2 | HIS | 82 | 137.002 | 29.989 | 32.553 | 1.00 | 7.90 |
| | 520 | ND1 | HIS | 82 | 136.574 | 30.742 | 30.548 | 1.00 | 14.62 |
| | 521 | CE1 | HIS | 82 | 136.829 | 31.788 | 31.312 | 1.00 | 11.77 |
| | 522 | NE2 | HIS | 82 | 137.091 | 31.359 | 32.533 | 1.00 | 13.85 |
| 30 | 523 | C | HIS | 82 | 135.085 | 26.654 | 29.440 | 1.00 | 28.78 |
| | 524 | O | HIS | 82 | 135.456 | 26.643 | 28.265 | 1.00 | 31.36 |
| | 525 | N | PHE | 83 | 134.719 | 25.557 | 30.098 | 1.00 | 30.57 |
| | 526 | CA | PHE | 83 | 134.774 | 24.241 | 29.475 | 1.00 | 32.99 |
| | 527 | CB | PHE | 83 | 135.829 | 23.389 | 30.191 | 1.00 | 38.74 |
| 35 | 528 | CG | PHE | 83 | 137.052 | 24.157 | 30.603 | 1.00 | 40.58 |
| | 529 | CD1 | PHE | 83 | 137.204 | 24.583 | 31.921 | 1.00 | 40.06 |
| | 530 | CD2 | PHE | 83 | 138.041 | 24.476 | 29.675 | 1.00 | 41.50 |
| | 531 | CE1 | PHE | 83 | 138.320 | 25.318 | 32.309 | 1.00 | 43.27 |
| | 532 | CE2 | PHE | 83 | 139.163 | 25.211 | 30.050 | 1.00 | 38.18 |
| 40 | 533 | CZ | PHE | 83 | 139.303 | 25.634 | 31.371 | 1.00 | 46.92 |
| | 534 | C | PHE | 83 | 133.444 | 23.496 | 29.471 | 1.00 | 32.87 |
| | 535 | O | PHE | 83 | 133.378 | 22.340 | 29.886 | 1.00 | 31.33 |
| | 536 | N | GLU | 84 | 132.397 | 24.133 | 28.960 | 1.00 | 33.76 |
| | 537 | CA | GLU | 84 | 131.086 | 23.496 | 28.929 | 1.00 | 38.03 |
| 45 | 538 | CB | GLU | 84 | 129.991 | 24.514 | 28.601 | 1.00 | 47.83 |
| | 539 | CG | GLU | 84 | 129.901 | 25.690 | 29.578 | 1.00 | 58.57 |
| | 540 | CD | GLU | 84 | 129.403 | 25.312 | 30.975 | 1.00 | 69.66 |
| | 541 | OE1 | GLU | 84 | 129.719 | 24.208 | 31.479 | 1.00 | 74.44 |
| | 542 | OE2 | GLU | 84 | 128.695 | 26.146 | 31.586 | 1.00 | 66.21 |
| 50 | 543 | C | GLU | 84 | 131.030 | 22.314 | 27.966 | 1.00 | 39.30 |

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|----|-----|-----|-----|----|---------|--------|--------|------|-------|
| | 544 | O | GLU | 84 | 130.339 | 21.328 | 28.228 | 1.00 | 37.93 |
| | 545 | N | LYS | 85 | 131.780 | 22.401 | 26.872 | 1.00 | 37.65 |
| | 546 | CA | LYS | 85 | 131.815 | 21.329 | 25.886 | 1.00 | 40.19 |
| 5 | 547 | CB | LYS | 85 | 132.367 | 21.839 | 24.551 | 1.00 | 49.51 |
| | 548 | CG | LYS | 85 | 132.443 | 20.770 | 23.469 | 1.00 | 57.11 |
| | 549 | CD | LYS | 85 | 133.176 | 21.261 | 22.237 | 1.00 | 73.34 |
| | 550 | CE | LYS | 85 | 133.280 | 20.160 | 21.180 | 1.00 | 81.58 |
| | 551 | NZ | LYS | 85 | 134.029 | 20.532 | 19.952 | 1.00 | 94.03 |
| 10 | 552 | C | LYS | 85 | 132.661 | 20.161 | 26.381 | 1.00 | 37.98 |
| | 553 | O | LYS | 85 | 132.200 | 19.018 | 26.404 | 1.00 | 43.86 |
| | 554 | N | GLU | 86 | 133.894 | 20.461 | 26.784 | 1.00 | 36.06 |
| | 555 | CA | GLU | 86 | 134.825 | 19.448 | 27.277 | 1.00 | 32.72 |
| | 556 | CB | GLU | 86 | 136.122 | 20.102 | 27.774 | 1.00 | 36.71 |
| 15 | 557 | CG | GLU | 86 | 136.998 | 20.743 | 26.698 | 1.00 | 42.45 |
| | 558 | CD | GLU | 86 | 136.500 | 22.103 | 26.219 | 1.00 | 44.54 |
| | 559 | OE1 | GLU | 86 | 135.646 | 22.720 | 26.891 | 1.00 | 49.68 |
| | 560 | OE2 | GLU | 86 | 136.977 | 22.566 | 25.162 | 1.00 | 47.77 |
| | 561 | C | GLU | 86 | 134.213 | 18.618 | 28.402 | 1.00 | 29.96 |
| 20 | 562 | O | GLU | 86 | 134.254 | 17.389 | 28.370 | 1.00 | 32.06 |
| | 563 | N | ILE | 87 | 133.638 | 19.303 | 29.388 | 1.00 | 28.21 |
| | 564 | CA | ILE | 87 | 133.013 | 18.648 | 30.534 | 1.00 | 27.11 |
| | 565 | CB | ILE | 87 | 132.618 | 19.672 | 31.617 | 1.00 | 28.37 |
| | 566 | CG2 | ILE | 87 | 131.813 | 18.996 | 32.729 | 1.00 | 28.34 |
| 25 | 567 | CG1 | ILE | 87 | 133.880 | 20.338 | 32.179 | 1.00 | 22.12 |
| | 568 | CD1 | ILE | 87 | 133.613 | 21.386 | 33.241 | 1.00 | 21.16 |
| | 569 | C | ILE | 87 | 131.795 | 17.815 | 30.150 | 1.00 | 27.00 |
| | 570 | O | ILE | 87 | 131.581 | 16.735 | 30.700 | 1.00 | 29.31 |
| | 571 | N | ASP | 88 | 131.007 | 18.309 | 29.200 | 1.00 | 31.52 |
| 30 | 572 | CA | ASP | 88 | 129.815 | 17.593 | 28.751 | 1.00 | 39.20 |
| | 573 | CB | ASP | 88 | 129.009 | 18.445 | 27.764 | 1.00 | 40.43 |
| | 574 | CG | ASP | 88 | 127.717 | 17.774 | 27.330 | 1.00 | 36.63 |
| | 575 | OD1 | ASP | 88 | 126.845 | 17.539 | 28.194 | 1.00 | 36.19 |
| | 576 | OD2 | ASP | 88 | 127.577 | 17.470 | 26.125 | 1.00 | 42.80 |
| 35 | 577 | C | ASP | 88 | 130.173 | 16.253 | 28.107 | 1.00 | 40.12 |
| | 578 | O | ASP | 88 | 129.660 | 15.210 | 28.513 | 1.00 | 41.11 |
| | 579 | N | ASP | 89 | 131.088 | 16.251 | 27.130 | 1.00 | 37.03 |
| | 580 | CA | ASP | 89 | 131.496 | 15.096 | 26.397 | 1.00 | 33.87 |
| | 581 | C | ASP | 89 | 132.107 | 14.047 | 27.304 | 1.00 | 33.85 |
| 40 | 582 | O | ASP | 89 | 132.047 | 12.832 | 26.978 | 1.00 | 33.37 |
| | 583 | CB | ASP | 89 | 132.464 | 15.574 | 25.325 | 1.00 | 27.32 |
| | 584 | CG | ASP | 89 | 131.779 | 16.561 | 24.391 | 1.00 | 34.13 |
| | 585 | OD1 | ASP | 89 | 130.528 | 16.553 | 24.341 | 1.00 | 20.00 |
| | 586 | OD2 | ASP | 89 | 132.481 | 17.345 | 23.721 | 1.00 | 20.00 |
| 45 | 587 | N | ILE | 90 | 132.765 | 14.453 | 28.372 | 1.00 | 31.52 |
| | 588 | CA | ILE | 90 | 133.385 | 13.527 | 29.308 | 1.00 | 25.50 |
| | 589 | CB | ILE | 90 | 134.370 | 14.245 | 30.258 | 1.00 | 22.28 |
| | 590 | CG2 | ILE | 90 | 134.861 | 13.285 | 31.328 | 1.00 | 22.91 |
| | 591 | CG1 | ILE | 90 | 135.549 | 14.818 | 29.465 | 1.00 | 31.26 |
| | 592 | CD1 | ILE | 90 | 136.543 | 15.620 | 30.301 | 1.00 | 31.23 |
| 50 | 593 | C | ILE | 90 | 132.297 | 12.836 | 30.124 | 1.00 | 23.61 |

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|----|-----|-----|-----|----|---------|--------|--------|------|-------|
| | 594 | O | ILE | 90 | 132.331 | 11.620 | 30.316 | 1.00 | 27.20 |
| | 595 | N | LEU | 91 | 131.331 | 13.622 | 30.593 | 1.00 | 23.72 |
| | 596 | CA | LEU | 91 | 130.218 | 13.099 | 31.379 | 1.00 | 20.80 |
| | 597 | CB | LEU | 91 | 129.469 | 14.238 | 32.071 | 1.00 | 20.19 |
| 5 | 598 | CG | LEU | 91 | 130.232 | 14.888 | 33.225 | 1.00 | 17.15 |
| | 599 | CD1 | LEU | 91 | 129.464 | 16.078 | 33.772 | 1.00 | 13.18 |
| | 600 | CD2 | LEU | 91 | 130.479 | 13.852 | 34.318 | 1.00 | 9.86 |
| | 601 | C | LEU | 91 | 129.270 | 12.281 | 30.510 | 1.00 | 22.03 |
| | 602 | O | LEU | 91 | 128.649 | 11.334 | 30.988 | 1.00 | 22.93 |
| 10 | 603 | N | ASP | 92 | 129.183 | 12.640 | 29.231 | 1.00 | 21.86 |
| | 604 | CA | ASP | 92 | 128.337 | 11.930 | 28.276 | 1.00 | 23.86 |
| | 605 | CB | ASP | 92 | 128.314 | 12.668 | 26.933 | 1.00 | 30.84 |
| | 606 | CG | ASP | 92 | 127.282 | 12.105 | 25.973 | 1.00 | 37.16 |
| | 607 | OD1 | ASP | 92 | 126.182 | 12.690 | 25.879 | 1.00 | 34.52 |
| 15 | 608 | OD2 | ASP | 92 | 127.568 | 11.083 | 25.309 | 1.00 | 45.02 |
| | 609 | C | ASP | 92 | 128.928 | 10.539 | 28.090 | 1.00 | 30.87 |
| | 610 | O | ASP | 92 | 128.208 | 9.542 | 28.106 | 1.00 | 38.64 |
| | 611 | N | GLN | 93 | 130.247 | 10.490 | 27.914 | 1.00 | 33.31 |
| | 612 | CA | GLN | 93 | 130.974 | 9.239 | 27.738 | 1.00 | 34.79 |
| 20 | 613 | CB | GLN | 93 | 132.454 | 9.531 | 27.466 | 1.00 | 46.61 |
| | 614 | CG | GLN | 93 | 133.345 | 8.300 | 27.331 | 1.00 | 60.12 |
| | 615 | CD | GLN | 93 | 134.831 | 8.640 | 27.354 | 1.00 | 75.57 |
| | 616 | OE1 | GLN | 93 | 135.217 | 9.801 | 27.510 | 1.00 | 79.60 |
| | 617 | NE2 | GLN | 93 | 135.672 | 7.621 | 27.208 | 1.00 | 81.92 |
| 25 | 618 | C | GLN | 93 | 130.833 | 8.380 | 28.994 | 1.00 | 35.74 |
| | 619 | O | GLN | 93 | 130.620 | 7.171 | 28.906 | 1.00 | 39.97 |
| | 620 | N | ILE | 94 | 130.933 | 9.019 | 30.159 | 1.00 | 32.85 |
| | 621 | CA | ILE | 94 | 130.817 | 8.326 | 31.441 | 1.00 | 35.57 |
| | 622 | CB | ILE | 94 | 131.191 | 9.266 | 32.625 | 1.00 | 33.17 |
| 30 | 623 | CG2 | ILE | 94 | 130.909 | 8.588 | 33.969 | 1.00 | 25.21 |
| | 624 | CG1 | ILE | 94 | 132.671 | 9.652 | 32.538 | 1.00 | 32.16 |
| | 625 | CD1 | ILE | 94 | 133.120 | 10.631 | 33.603 | 1.00 | 32.74 |
| | 626 | C | ILE | 94 | 129.407 | 7.770 | 31.645 | 1.00 | 38.37 |
| | 627 | O | ILE | 94 | 129.224 | 6.716 | 32.260 | 1.00 | 45.31 |
| 35 | 628 | N | TYR | 95 | 128.421 | 8.477 | 31.102 | 1.00 | 38.86 |
| | 629 | CA | TYR | 95 | 127.021 | 8.082 | 31.212 | 1.00 | 39.68 |
| | 630 | CB | TYR | 95 | 126.122 | 9.249 | 30.784 | 1.00 | 34.17 |
| | 631 | CG | TYR | 95 | 124.637 | 8.974 | 30.877 | 1.00 | 27.88 |
| | 632 | CD1 | TYR | 95 | 124.060 | 8.539 | 32.070 | 1.00 | 26.18 |
| 40 | 633 | CE1 | TYR | 95 | 122.697 | 8.279 | 32.155 | 1.00 | 24.69 |
| | 634 | CD2 | TYR | 95 | 123.810 | 9.144 | 29.770 | 1.00 | 21.67 |
| | 635 | CE2 | TYR | 95 | 122.447 | 8.888 | 29.845 | 1.00 | 22.88 |
| | 636 | CZ | TYR | 95 | 121.896 | 8.454 | 31.039 | 1.00 | 23.25 |
| | 637 | OH | TYR | 95 | 120.546 | 8.185 | 31.112 | 1.00 | 32.19 |
| 45 | 638 | C | TYR | 95 | 126.715 | 6.846 | 30.369 | 1.00 | 40.10 |
| | 639 | O | TYR | 95 | 125.987 | 5.953 | 30.803 | 1.00 | 41.67 |
| | 640 | N | ASN | 96 | 127.291 | 6.796 | 29.173 | 1.00 | 40.40 |
| | 641 | CA | ASN | 96 | 127.073 | 5.682 | 28.261 | 1.00 | 50.10 |
| | 642 | CB | ASN | 96 | 127.273 | 6.146 | 26.815 | 1.00 | 50.46 |
| 50 | 643 | CG | ASN | 96 | 126.252 | 7.189 | 26.392 | 1.00 | 53.74 |

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|----|-----|-----|-----|-----|---------|--------|--------|------|--------|
| | 644 | OD1 | ASN | 96 | 125.093 | 7.141 | 26.806 | 1.00 | 52.90 |
| | 645 | ND2 | ASN | 96 | 126.679 | 8.138 | 25.567 | 1.00 | 56.55 |
| | 646 | C | ASN | 96 | 127.911 | 4.434 | 28.545 | 1.00 | 54.46 |
| | 647 | O | ASN | 96 | 127.502 | 3.324 | 28.202 | 1.00 | 58.60 |
| 5 | 648 | N | GLN | 97 | 129.067 | 4.606 | 29.183 | 1.00 | 57.00 |
| | 649 | CA | GLN | 97 | 129.933 | 3.469 | 29.494 | 1.00 | 62.35 |
| | 650 | CB | GLN | 97 | 131.385 | 3.924 | 29.690 | 1.00 | 63.17 |
| | 651 | CG | GLN | 97 | 131.622 | 4.834 | 30.885 | 1.00 | 68.59 |
| | 652 | CD | GLN | 97 | 133.052 | 5.351 | 30.970 | 1.00 | 68.54 |
| 10 | 653 | OE1 | GLN | 97 | 133.659 | 5.357 | 32.040 | 1.00 | 66.32 |
| | 654 | NE2 | GLN | 97 | 133.594 | 5.798 | 29.836 | 1.00 | 59.07 |
| | 655 | C | GLN | 97 | 129.458 | 2.654 | 30.698 | 1.00 | 66.41 |
| | 656 | O | GLN | 97 | 129.682 | 1.442 | 30.754 | 1.00 | 66.29 |
| | 657 | N | ASN | 98 | 128.790 | 3.317 | 31.642 | 1.00 | 75.07 |
| 15 | 658 | CA | ASN | 98 | 128.274 | 2.676 | 32.854 | 1.00 | 85.32 |
| | 659 | CB | ASN | 98 | 127.000 | 1.878 | 32.554 | 1.00 | 92.56 |
| | 660 | CG | ASN | 98 | 125.798 | 2.771 | 32.325 | 1.00 | 97.44 |
| | 661 | OD1 | ASN | 98 | 125.273 | 3.375 | 33.262 | 1.00 | 97.63 |
| | 662 | ND2 | ASN | 98 | 125.357 | 2.865 | 31.074 | 1.00 | 98.68 |
| 20 | 663 | C | ASN | 98 | 129.314 | 1.791 | 33.535 | 1.00 | 89.40 |
| | 664 | O | ASN | 98 | 129.073 | 0.612 | 33.812 | 1.00 | 88.19 |
| | 665 | N | SER | 99 | 130.486 | 2.369 | 33.779 | 1.00 | 94.53 |
| | 666 | CA | SER | 99 | 131.560 | 1.640 | 34.435 | 1.00 | 98.60 |
| | 667 | CB | SER | 99 | 132.918 | 2.248 | 34.106 | 1.00 | 99.63 |
| 25 | 668 | OG | SER | 99 | 132.996 | 3.591 | 34.559 | 1.00 | 100.00 |
| | 669 | C | SER | 99 | 131.332 | 1.673 | 35.926 | 1.00 | 99.96 |
| | 670 | O | SER | 99 | 131.030 | 2.717 | 36.500 | 1.00 | 98.72 |
| | 671 | N | ASN | 100 | 131.508 | 0.532 | 36.566 | 1.00 | 100.00 |
| | 672 | CA | ASN | 100 | 131.294 | 0.473 | 37.995 | 1.00 | 100.00 |
| 30 | 673 | CB | ASN | 100 | 130.733 | -0.892 | 38.382 | 1.00 | 97.11 |
| | 674 | CG | ASN | 100 | 129.297 | -1.056 | 37.956 | 1.00 | 95.75 |
| | 675 | OD1 | ASN | 100 | 128.429 | -0.279 | 38.360 | 1.00 | 86.86 |
| | 676 | ND2 | ASN | 100 | 129.028 | -2.069 | 37.139 | 1.00 | 94.51 |
| | 677 | C | ASN | 100 | 132.513 | 0.784 | 38.857 | 1.00 | 100.00 |
| 35 | 678 | O | ASN | 100 | 133.196 | -0.133 | 39.303 | 1.00 | 100.00 |
| | 679 | N | CYS | 101 | 132.829 | 2.068 | 39.047 | 1.00 | 98.98 |
| | 680 | CA | CYS | 101 | 133.942 | 2.429 | 39.953 | 1.00 | 94.29 |
| | 681 | CB | CYS | 101 | 134.350 | 3.905 | 39.872 | 1.00 | 96.36 |
| | 682 | SG | CYS | 101 | 135.708 | 4.382 | 41.017 | 1.00 | 100.00 |
| 40 | 683 | C | CYS | 101 | 133.151 | 2.160 | 41.226 | 1.00 | 90.03 |
| | 684 | O | CYS | 101 | 132.261 | 2.914 | 41.595 | 1.00 | 89.78 |
| | 685 | N | ASN | 102 | 133.483 | 1.057 | 41.870 | 1.00 | 85.97 |
| | 686 | CA | ASN | 102 | 132.753 | 0.573 | 43.043 | 1.00 | 81.73 |
| | 687 | CB | ASN | 102 | 133.072 | -0.902 | 43.238 | 1.00 | 86.41 |
| 45 | 688 | CG | ASN | 102 | 132.971 | -1.688 | 41.962 | 1.00 | 88.71 |
| | 689 | OD1 | ASN | 102 | 133.978 | -2.107 | 41.412 | 1.00 | 90.82 |
| | 690 | ND2 | ASN | 102 | 131.750 | -1.869 | 41.462 | 1.00 | 81.79 |
| | 691 | C | ASN | 102 | 132.652 | 1.257 | 44.413 | 1.00 | 74.07 |
| | 692 | O | ASN | 102 | 131.770 | 0.881 | 45.187 | 1.00 | 77.40 |
| 50 | 693 | N | ASP | 103 | 133.474 | 2.260 | 44.713 | 1.00 | 58.82 |

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|----|-----|-----|-----|-----|---------|--------|--------|------|-------|
| | 694 | CA | ASP | 103 | 133.377 | 2.904 | 46.037 | 1.00 | 48.91 |
| | 695 | CB | ASP | 103 | 134.746 | 3.418 | 46.524 | 1.00 | 50.06 |
| | 696 | CG | ASP | 103 | 135.346 | 4.487 | 45.622 | 1.00 | 54.31 |
| | 697 | OD1 | ASP | 103 | 135.589 | 4.210 | 44.429 | 1.00 | 68.60 |
| 5 | 698 | OD2 | ASP | 103 | 135.616 | 5.599 | 46.128 | 1.00 | 47.23 |
| | 699 | C | ASP | 103 | 132.290 | 3.974 | 46.178 | 1.00 | 38.98 |
| | 700 | O | ASP | 103 | 131.875 | 4.585 | 45.198 | 1.00 | 30.42 |
| | 701 | N | LEU | 104 | 131.820 | 4.168 | 47.408 | 1.00 | 25.79 |
| | 702 | CA | LEU | 104 | 130.764 | 5.139 | 47.702 | 1.00 | 26.09 |
| 10 | 703 | CB | LEU | 104 | 130.414 | 5.114 | 49.195 | 1.00 | 14.86 |
| | 704 | CG | LEU | 104 | 129.294 | 6.042 | 49.674 | 1.00 | 13.82 |
| | 705 | CD1 | LEU | 104 | 127.971 | 5.654 | 49.031 | 1.00 | 10.36 |
| | 706 | CD2 | LEU | 104 | 129.171 | 5.996 | 51.191 | 1.00 | 7.52 |
| | 707 | C | LEU | 104 | 131.082 | 6.567 | 47.274 | 1.00 | 26.59 |
| 15 | 708 | O | LEU | 104 | 130.232 | 7.240 | 46.696 | 1.00 | 27.23 |
| | 709 | N | CYS | 105 | 132.297 | 7.021 | 47.574 | 1.00 | 28.20 |
| | 710 | CA | CYS | 105 | 132.735 | 8.370 | 47.225 | 1.00 | 24.21 |
| | 711 | CB | CYS | 105 | 134.164 | 8.606 | 47.721 | 1.00 | 29.54 |
| | 712 | SG | CYS | 105 | 134.889 | 10.178 | 47.188 | 1.00 | 32.14 |
| 20 | 713 | C | CYS | 105 | 132.659 | 8.634 | 45.724 | 1.00 | 20.98 |
| | 714 | O | CYS | 105 | 132.062 | 9.618 | 45.285 | 1.00 | 24.94 |
| | 715 | N | THR | 106 | 133.258 | 7.744 | 44.941 | 1.00 | 22.03 |
| | 716 | CA | THR | 106 | 133.261 | 7.890 | 43.489 | 1.00 | 23.52 |
| | 717 | CB | THR | 106 | 134.197 | 6.858 | 42.823 | 1.00 | 18.21 |
| 25 | 718 | OG1 | THR | 106 | 135.481 | 6.893 | 43.461 | 1.00 | 20.18 |
| | 719 | CG2 | THR | 106 | 134.372 | 7.183 | 41.349 | 1.00 | 18.22 |
| | 720 | C | THR | 106 | 131.858 | 7.739 | 42.906 | 1.00 | 22.72 |
| | 721 | O | THR | 106 | 131.481 | 8.465 | 41.984 | 1.00 | 21.14 |
| | 722 | N | SER | 107 | 131.092 | 6.802 | 43.461 | 1.00 | 26.53 |
| 30 | 723 | CA | SER | 107 | 129.730 | 6.532 | 43.009 | 1.00 | 24.15 |
| | 724 | CB | SER | 107 | 129.158 | 5.312 | 43.735 | 1.00 | 24.72 |
| | 725 | OG | SER | 107 | 129.913 | 4.147 | 43.453 | 1.00 | 34.14 |
| | 726 | C | SER | 107 | 128.818 | 7.731 | 43.228 | 1.00 | 20.49 |
| | 727 | O | SER | 107 | 128.128 | 8.170 | 42.306 | 1.00 | 15.26 |
| 35 | 728 | N | ALA | 108 | 128.822 | 8.254 | 44.453 | 1.00 | 18.95 |
| | 729 | CA | ALA | 108 | 128.002 | 9.408 | 44.810 | 1.00 | 16.79 |
| | 730 | CB | ALA | 108 | 128.168 | 9.732 | 46.282 | 1.00 | 13.84 |
| | 731 | C | ALA | 108 | 128.349 | 10.623 | 43.953 | 1.00 | 15.33 |
| | 732 | O | ALA | 108 | 127.455 | 11.340 | 43.499 | 1.00 | 19.47 |
| 40 | 733 | N | LEU | 109 | 129.644 | 10.836 | 43.722 | 1.00 | 10.72 |
| | 734 | CA | LEU | 109 | 130.106 | 11.954 | 42.907 | 1.00 | 11.35 |
| | 735 | CB | LEU | 109 | 131.627 | 12.093 | 42.993 | 1.00 | 15.00 |
| | 736 | CG | LEU | 109 | 132.277 | 13.237 | 42.203 | 1.00 | 19.48 |
| | 737 | CD1 | LEU | 109 | 131.670 | 14.577 | 42.596 | 1.00 | 15.00 |
| 45 | 738 | CD2 | LEU | 109 | 133.778 | 13.239 | 42.442 | 1.00 | 17.22 |
| | 739 | C | LEU | 109 | 129.673 | 11.754 | 41.459 | 1.00 | 15.76 |
| | 740 | O | LEU | 109 | 129.216 | 12.692 | 40.807 | 1.00 | 28.55 |
| | 741 | N | GLN | 110 | 129.813 | 10.526 | 40.966 | 1.00 | 19.50 |
| | 742 | CA | GLN | 110 | 129.417 | 10.184 | 39.600 | 1.00 | 20.50 |
| 50 | 743 | CB | GLN | 110 | 129.679 | 8.699 | 39.339 | 1.00 | 24.06 |

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|----|-----|-----|-----|-----|---------|--------|--------|------|-------|
| | 744 | CG | GLN | 110 | 129.287 | 8.221 | 37.949 | 1.00 | 31.51 |
| | 745 | CD | GLN | 110 | 129.373 | 6.711 | 37.797 | 1.00 | 31.57 |
| | 746 | OE1 | GLN | 110 | 129.661 | 5.990 | 38.756 | 1.00 | 35.16 |
| | 747 | NE2 | GLN | 110 | 129.117 | 6.225 | 36.586 | 1.00 | 34.19 |
| 5 | 748 | C | GLN | 110 | 127.926 | 10.478 | 39.414 | 1.00 | 21.12 |
| | 749 | O | GLN | 110 | 127.508 | 11.009 | 38.389 | 1.00 | 20.13 |
| | 750 | N | PHE | 111 | 127.139 | 10.140 | 40.431 | 1.00 | 23.63 |
| | 751 | CA | PHE | 111 | 125.699 | 10.356 | 40.409 | 1.00 | 21.06 |
| | 752 | CB | PHE | 111 | 125.065 | 9.729 | 41.655 | 1.00 | 21.44 |
| 10 | 753 | CG | PHE | 111 | 123.565 | 9.806 | 41.685 | 1.00 | 18.29 |
| | 754 | CD1 | PHE | 111 | 122.795 | 8.933 | 40.924 | 1.00 | 18.70 |
| | 755 | CD2 | PHE | 111 | 122.921 | 10.744 | 42.483 | 1.00 | 14.43 |
| | 756 | CE1 | PHE | 111 | 121.404 | 8.990 | 40.959 | 1.00 | 18.31 |
| | 757 | CE2 | PHE | 111 | 121.533 | 10.810 | 42.523 | 1.00 | 21.91 |
| 15 | 758 | CZ | PHE | 111 | 120.773 | 9.929 | 41.758 | 1.00 | 17.47 |
| | 759 | C | PHE | 111 | 125.373 | 11.846 | 40.345 | 1.00 | 19.49 |
| | 760 | O | PHE | 111 | 124.731 | 12.305 | 39.399 | 1.00 | 17.88 |
| | 761 | N | ARG | 112 | 125.857 | 12.598 | 41.332 | 1.00 | 16.34 |
| | 762 | CA | ARG | 112 | 125.606 | 14.033 | 41.407 | 1.00 | 8.21 |
| 20 | 763 | CB | ARG | 112 | 126.326 | 14.651 | 42.608 | 1.00 | 7.94 |
| | 764 | CG | ARG | 112 | 126.081 | 16.153 | 42.745 | 1.00 | 14.61 |
| | 765 | CD | ARG | 112 | 126.507 | 16.703 | 44.100 | 1.00 | 22.36 |
| | 766 | NE | ARG | 112 | 127.955 | 16.745 | 44.291 | 1.00 | 19.69 |
| | 767 | CZ | ARG | 112 | 128.777 | 17.561 | 43.639 | 1.00 | 22.41 |
| 25 | 768 | NH1 | ARG | 112 | 128.300 | 18.407 | 42.737 | 1.00 | 29.76 |
| | 769 | NH2 | ARG | 112 | 130.073 | 17.555 | 43.915 | 1.00 | 26.92 |
| | 770 | C | ARG | 112 | 125.961 | 14.808 | 40.145 | 1.00 | 13.57 |
| | 771 | O | ARG | 112 | 125.113 | 15.505 | 39.588 | 1.00 | 17.92 |
| | 772 | N | LEU | 113 | 127.205 | 14.676 | 39.693 | 1.00 | 11.94 |
| 30 | 773 | CA | LEU | 113 | 127.671 | 15.385 | 38.504 | 1.00 | 14.83 |
| | 774 | CB | LEU | 113 | 129.151 | 15.088 | 38.239 | 1.00 | 20.65 |
| | 775 | CG | LEU | 113 | 130.149 | 15.516 | 39.322 | 1.00 | 16.72 |
| | 776 | CD1 | LEU | 113 | 131.568 | 15.259 | 38.847 | 1.00 | 15.77 |
| | 777 | CD2 | LEU | 113 | 129.970 | 16.985 | 39.651 | 1.00 | 21.06 |
| 35 | 778 | C | LEU | 113 | 126.840 | 15.108 | 37.256 | 1.00 | 19.17 |
| | 779 | O | LEU | 113 | 126.484 | 16.034 | 36.532 | 1.00 | 26.79 |
| | 780 | N | LEU | 114 | 126.516 | 13.841 | 37.014 | 1.00 | 23.83 |
| | 781 | CA | LEU | 114 | 125.717 | 13.464 | 35.849 | 1.00 | 14.66 |
| | 782 | CB | LEU | 114 | 125.668 | 11.943 | 35.703 | 1.00 | 18.52 |
| 40 | 783 | CG | LEU | 114 | 126.969 | 11.251 | 35.287 | 1.00 | 19.65 |
| | 784 | CD1 | LEU | 114 | 126.800 | 9.746 | 35.362 | 1.00 | 22.06 |
| | 785 | CD2 | LEU | 114 | 127.352 | 11.666 | 33.882 | 1.00 | 21.06 |
| | 786 | C | LEU | 114 | 124.300 | 14.030 | 35.939 | 1.00 | 15.67 |
| | 787 | O | LEU | 114 | 123.787 | 14.596 | 34.972 | 1.00 | 18.67 |
| 45 | 788 | N | ARG | 115 | 123.678 | 13.883 | 37.104 | 1.00 | 9.26 |
| | 789 | CA | ARG | 115 | 122.328 | 14.387 | 37.328 | 1.00 | 7.86 |
| | 790 | CB | ARG | 115 | 121.849 | 14.021 | 38.736 | 1.00 | 10.49 |
| | 791 | CG | ARG | 115 | 121.450 | 12.562 | 38.901 | 1.00 | 12.35 |
| | 792 | CD | ARG | 115 | 120.323 | 12.202 | 37.949 | 1.00 | 17.12 |
| 50 | 793 | NE | ARG | 115 | 119.807 | 10.857 | 38.179 | 1.00 | 21.26 |

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|----|-----|-----|-----|-----|---------|--------|--------|------|-------|
| | 794 | CZ | ARG | 115 | 118.803 | 10.570 | 39.000 | 1.00 | 15.94 |
| | 795 | NH1 | ARG | 115 | 118.199 | 11.537 | 39.676 | 1.00 | 8.20 |
| | 796 | NH2 | ARG | 115 | 118.406 | 9.314 | 39.152 | 1.00 | 17.38 |
| 5 | 797 | C | ARG | 115 | 122.250 | 15.899 | 37.126 | 1.00 | 13.44 |
| | 798 | O | ARG | 115 | 121.379 | 16.390 | 36.402 | 1.00 | 8.27 |
| | 799 | N | GLN | 116 | 123.180 | 16.629 | 37.743 | 1.00 | 14.35 |
| | 800 | CA | GLN | 116 | 123.225 | 18.086 | 37.629 | 1.00 | 11.93 |
| | 801 | CB | GLN | 116 | 124.364 | 18.664 | 38.471 | 1.00 | 4.12 |
| 10 | 802 | CG | GLN | 116 | 124.165 | 18.534 | 39.968 | 1.00 | 5.13 |
| | 803 | CD | GLN | 116 | 125.303 | 19.142 | 40.768 | 1.00 | 11.78 |
| | 804 | OE1 | GLN | 116 | 125.080 | 19.950 | 41.669 | 1.00 | 21.37 |
| | 805 | NE2 | GLN | 116 | 126.530 | 18.747 | 40.451 | 1.00 | 11.47 |
| | 806 | C | GLN | 116 | 123.392 | 18.530 | 36.183 | 1.00 | 15.48 |
| 15 | 807 | O | GLN | 116 | 123.126 | 19.682 | 35.851 | 1.00 | 19.88 |
| | 808 | N | HIS | 117 | 123.827 | 17.607 | 35.328 | 1.00 | 19.55 |
| | 809 | CA | HIS | 117 | 124.031 | 17.893 | 33.912 | 1.00 | 15.02 |
| | 810 | CB | HIS | 117 | 125.405 | 17.392 | 33.460 | 1.00 | 13.78 |
| | 811 | CG | HIS | 117 | 126.538 | 18.253 | 33.925 | 1.00 | 17.44 |
| 20 | 812 | CD2 | HIS | 117 | 126.999 | 18.525 | 35.169 | 1.00 | 18.38 |
| | 813 | ND1 | HIS | 117 | 127.322 | 18.983 | 33.059 | 1.00 | 19.26 |
| | 814 | CE1 | HIS | 117 | 128.216 | 19.668 | 33.748 | 1.00 | 20.36 |
| | 815 | NE2 | HIS | 117 | 128.042 | 19.408 | 35.031 | 1.00 | 17.37 |
| | 816 | C | HIS | 117 | 122.930 | 17.349 | 33.006 | 1.00 | 16.42 |
| 25 | 817 | O | HIS | 117 | 123.036 | 17.419 | 31.780 | 1.00 | 15.29 |
| | 818 | N | GLY | 118 | 121.872 | 16.813 | 33.613 | 1.00 | 17.98 |
| | 819 | CA | GLY | 118 | 120.756 | 16.292 | 32.839 | 1.00 | 21.36 |
| | 820 | C | GLY | 118 | 120.761 | 14.808 | 32.521 | 1.00 | 21.11 |
| | 821 | O | GLY | 118 | 119.760 | 14.284 | 32.032 | 1.00 | 23.89 |
| 30 | 822 | N | PHE | 119 | 121.880 | 14.134 | 32.773 | 1.00 | 20.97 |
| | 823 | CA | PHE | 119 | 121.994 | 12.702 | 32.510 | 1.00 | 15.97 |
| | 824 | CB | PHE | 119 | 123.465 | 12.282 | 32.477 | 1.00 | 13.26 |
| | 825 | CG | PHE | 119 | 124.281 | 13.007 | 31.439 | 1.00 | 19.34 |
| | 826 | CD1 | PHE | 119 | 125.155 | 14.025 | 31.808 | 1.00 | 18.10 |
| 35 | 827 | CD2 | PHE | 119 | 124.160 | 12.686 | 30.090 | 1.00 | 17.78 |
| | 828 | CE1 | PHE | 119 | 125.896 | 14.714 | 30.850 | 1.00 | 14.61 |
| | 829 | CE2 | PHE | 119 | 124.896 | 13.370 | 29.122 | 1.00 | 16.11 |
| | 830 | CZ | PHE | 119 | 125.765 | 14.386 | 29.503 | 1.00 | 22.05 |
| | 831 | C | PHE | 119 | 121.238 | 11.917 | 33.576 | 1.00 | 20.90 |
| 40 | 832 | O | PHE | 119 | 121.620 | 11.910 | 34.749 | 1.00 | 17.99 |
| | 833 | N | ASN | 120 | 120.157 | 11.263 | 33.161 | 1.00 | 20.78 |
| | 834 | CA | ASN | 120 | 119.326 | 10.494 | 34.078 | 1.00 | 23.46 |
| | 835 | CB | ASN | 120 | 117.928 | 10.307 | 33.477 | 1.00 | 23.75 |
| | 836 | CG | ASN | 120 | 116.919 | 9.766 | 34.481 | 1.00 | 23.50 |
| | 837 | OD1 | ASN | 120 | 117.147 | 9.782 | 35.695 | 1.00 | 18.94 |
| 45 | 838 | ND2 | ASN | 120 | 115.786 | 9.295 | 33.973 | 1.00 | 24.72 |
| | 839 | C | ASN | 120 | 119.940 | 9.145 | 34.447 | 1.00 | 29.37 |
| | 840 | O | ASN | 120 | 119.467 | 8.092 | 34.011 | 1.00 | 37.56 |
| | 841 | N | ILE | 121 | 120.999 | 9.183 | 35.251 | 1.00 | 30.57 |
| 50 | 842 | CA | ILE | 121 | 121.674 | 7.965 | 35.691 | 1.00 | 28.30 |
| | 843 | CB | ILE | 121 | 123.118 | 8.250 | 36.202 | 1.00 | 31.51 |

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|----|-----|-----|-----|-----|---------|--------|--------|------|-------|
| | 844 | CG2 | ILE | 121 | 123.116 | 9.395 | 37.212 | 1.00 | 18.33 |
| | 845 | CG1 | ILE | 121 | 123.734 | 6.970 | 36.784 | 1.00 | 34.25 |
| | 846 | CD1 | ILE | 121 | 125.160 | 7.119 | 37.270 | 1.00 | 35.18 |
| 5 | 847 | C | ILE | 121 | 120.862 | 7.263 | 36.774 | 1.00 | 24.20 |
| | 848 | O | ILE | 121 | 120.435 | 7.888 | 37.746 | 1.00 | 29.58 |
| | 849 | N | SER | 122 | 120.654 | 5.963 | 36.594 | 1.00 | 28.31 |
| | 850 | CA | SER | 122 | 119.886 | 5.158 | 37.538 | 1.00 | 31.22 |
| | 851 | CB | SER | 122 | 119.782 | 3.711 | 37.040 | 1.00 | 37.94 |
| 10 | 852 | OG | SER | 122 | 119.046 | 2.907 | 37.948 | 1.00 | 37.31 |
| | 853 | C | SER | 122 | 120.471 | 5.193 | 38.942 | 1.00 | 26.25 |
| | 854 | O | SER | 122 | 121.690 | 5.086 | 39.121 | 1.00 | 36.49 |
| | 855 | N | PRO | 123 | 119.606 | 5.367 | 39.956 | 1.00 | 25.72 |
| | 856 | CD | PRO | 123 | 118.162 | 5.626 | 39.787 | 1.00 | 24.10 |
| | 857 | CA | PRO | 123 | 119.995 | 5.427 | 41.367 | 1.00 | 24.12 |
| 15 | 858 | CB | PRO | 123 | 118.807 | 6.139 | 42.015 | 1.00 | 14.52 |
| | 859 | CG | PRO | 123 | 117.635 | 5.620 | 41.222 | 1.00 | 18.26 |
| | 860 | C | PRO | 123 | 120.266 | 4.057 | 41.978 | 1.00 | 26.29 |
| | 861 | O | PRO | 123 | 120.649 | 3.957 | 43.143 | 1.00 | 26.93 |
| 20 | 862 | N | GLU | 124 | 120.106 | 3.007 | 41.176 | 1.00 | 31.58 |
| | 863 | CA | GLU | 124 | 120.362 | 1.656 | 41.665 | 1.00 | 42.38 |
| | 864 | CB | GLU | 124 | 119.734 | 0.614 | 40.749 | 1.00 | 52.63 |
| | 865 | CG | GLU | 124 | 118.661 | -0.182 | 41.472 | 1.00 | 66.87 |
| | 866 | CD | GLU | 124 | 117.857 | -1.078 | 40.558 | 1.00 | 84.70 |
| | 867 | OE1 | GLU | 124 | 118.072 | -1.045 | 39.323 | 1.00 | 92.92 |
| 25 | 868 | OE2 | GLU | 124 | 116.995 | -1.820 | 41.075 | 1.00 | 95.72 |
| | 869 | C | GLU | 124 | 121.850 | 1.396 | 41.860 | 1.00 | 40.43 |
| | 870 | O | GLU | 124 | 122.243 | 0.345 | 42.359 | 1.00 | 40.69 |
| | 871 | N | ILE | 125 | 122.665 | 2.383 | 41.493 | 1.00 | 40.56 |
| 30 | 872 | CA | ILE | 125 | 124.113 | 2.311 | 41.658 | 1.00 | 33.74 |
| | 873 | CB | ILE | 125 | 124.796 | 3.532 | 40.995 | 1.00 | 34.47 |
| | 874 | CG2 | ILE | 125 | 124.231 | 4.828 | 41.567 | 1.00 | 35.94 |
| | 875 | CG1 | ILE | 125 | 126.317 | 3.471 | 41.176 | 1.00 | 33.47 |
| | 876 | CD1 | ILE | 125 | 127.051 | 4.648 | 40.560 | 1.00 | 33.54 |
| | 877 | C | ILE | 125 | 124.397 | 2.311 | 43.166 | 1.00 | 27.96 |
| 35 | 878 | O | ILE | 125 | 125.450 | 1.867 | 43.612 | 1.00 | 32.46 |
| | 879 | N | PHE | 126 | 123.422 | 2.783 | 43.938 | 1.00 | 24.55 |
| | 880 | CA | PHE | 126 | 123.518 | 2.850 | 45.393 | 1.00 | 31.56 |
| | 881 | CB | PHE | 126 | 122.701 | 4.034 | 45.925 | 1.00 | 31.55 |
| 40 | 882 | CG | PHE | 126 | 123.245 | 5.377 | 45.536 | 1.00 | 36.38 |
| | 883 | CD1 | PHE | 126 | 122.701 | 6.079 | 44.465 | 1.00 | 32.78 |
| | 884 | CD2 | PHE | 126 | 124.300 | 5.946 | 46.245 | 1.00 | 35.39 |
| | 885 | CE1 | PHE | 126 | 123.197 | 7.328 | 44.105 | 1.00 | 32.25 |
| | 886 | CE2 | PHE | 126 | 124.805 | 7.194 | 45.894 | 1.00 | 31.56 |
| | 887 | CZ | PHE | 126 | 124.252 | 7.889 | 44.820 | 1.00 | 28.07 |
| 45 | 888 | C | PHE | 126 | 123.042 | 1.568 | 46.079 | 1.00 | 37.75 |
| | 889 | O | PHE | 126 | 122.939 | 1.520 | 47.308 | 1.00 | 36.32 |
| | 890 | N | SER | 127 | 122.730 | 0.542 | 45.289 | 1.00 | 42.49 |
| | 891 | CA | SER | 127 | 122.268 | -0.732 | 45.836 | 1.00 | 43.38 |
| | 892 | CB | SER | 127 | 121.659 | -1.601 | 44.733 | 1.00 | 48.30 |
| 50 | 893 | OG | SER | 127 | 120.465 | -1.025 | 44.233 | 1.00 | 59.77 |

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|----|-----|-----|-----|-----|---------|--------|--------|------|--------|
| | 894 | C | SER | 127 | 123.401 | -1.482 | 46.527 | 1.00 | 39.67 |
| | 895 | O | SER | 127 | 123.228 | -2.001 | 47.632 | 1.00 | 35.01 |
| | 896 | N | LYS | 128 | 124.567 | -1.503 | 45.886 | 1.00 | 35.16 |
| 5 | 897 | CA | LYS | 128 | 125.743 | -2.179 | 46.426 | 1.00 | 36.47 |
| | 898 | CB | LYS | 128 | 126.877 | -2.180 | 45.389 | 1.00 | 33.52 |
| | 899 | CG | LYS | 128 | 127.146 | -0.834 | 44.732 | 1.00 | 37.85 |
| | 900 | CD | LYS | 128 | 128.170 | -0.947 | 43.606 | 1.00 | 37.35 |
| | 901 | CE | LYS | 128 | 128.353 | 0.388 | 42.892 | 1.00 | 50.12 |
| 10 | 902 | NZ | LYS | 128 | 129.338 | 0.328 | 41.776 | 1.00 | 54.36 |
| | 903 | C | LYS | 128 | 126.233 | -1.623 | 47.769 | 1.00 | 38.71 |
| | 904 | O | LYS | 128 | 127.102 | -2.217 | 48.412 | 1.00 | 46.49 |
| | 905 | N | PHE | 129 | 125.656 | -0.501 | 48.199 | 1.00 | 38.63 |
| | 906 | CA | PHE | 129 | 126.028 | 0.135 | 49.466 | 1.00 | 31.98 |
| | 907 | CB | PHE | 129 | 126.309 | 1.626 | 49.256 | 1.00 | 24.98 |
| 15 | 908 | CG | PHE | 129 | 127.324 | 1.904 | 48.191 | 1.00 | 20.86 |
| | 909 | CD1 | PHE | 129 | 126.946 | 2.506 | 46.997 | 1.00 | 19.33 |
| | 910 | CD2 | PHE | 129 | 128.653 | 1.537 | 48.368 | 1.00 | 17.79 |
| | 911 | CE1 | PHE | 129 | 127.877 | 2.735 | 45.988 | 1.00 | 22.73 |
| | 912 | CE2 | PHE | 129 | 129.590 | 1.760 | 47.368 | 1.00 | 19.77 |
| 20 | 913 | CZ | PHE | 129 | 129.201 | 2.361 | 46.174 | 1.00 | 17.69 |
| | 914 | C | PHE | 129 | 124.929 | -0.024 | 50.509 | 1.00 | 31.84 |
| | 915 | O | PHE | 129 | 125.051 | 0.462 | 51.635 | 1.00 | 32.60 |
| | 916 | N | GLN | 130 | 123.854 | -0.700 | 50.123 | 1.00 | 40.45 |
| | 917 | CA | GLN | 130 | 122.720 | -0.922 | 51.010 | 1.00 | 47.58 |
| 25 | 918 | CB | GLN | 130 | 121.456 | -0.310 | 50.403 | 1.00 | 51.16 |
| | 919 | CG | GLN | 130 | 121.515 | 1.197 | 50.231 | 1.00 | 50.70 |
| | 920 | CD | GLN | 130 | 120.308 | 1.755 | 49.505 | 1.00 | 54.25 |
| | 921 | OE1 | GLN | 130 | 119.310 | 1.063 | 49.303 | 1.00 | 62.26 |
| | 922 | NE2 | GLN | 130 | 120.394 | 3.017 | 49.105 | 1.00 | 58.79 |
| 30 | 923 | C | GLN | 130 | 122.496 | -2.405 | 51.263 | 1.00 | 51.99 |
| | 924 | O | GLN | 130 | 122.818 | -3.245 | 50.419 | 1.00 | 55.44 |
| | 925 | N | ASP | 131 | 121.945 | -2.723 | 52.431 | 1.00 | 53.38 |
| | 926 | CA | ASP | 131 | 121.665 | -4.108 | 52.789 | 1.00 | 60.28 |
| | 927 | CB | ASP | 131 | 121.556 | -4.258 | 54.314 | 1.00 | 58.61 |
| 35 | 928 | CG | ASP | 131 | 120.311 | -3.596 | 54.892 | 1.00 | 62.05 |
| | 929 | OD1 | ASP | 131 | 119.749 | -4.145 | 55.860 | 1.00 | 69.31 |
| | 930 | OD2 | ASP | 131 | 119.893 | -2.532 | 54.391 | 1.00 | 65.85 |
| | 931 | C | ASP | 131 | 120.382 | -4.583 | 52.103 | 1.00 | 64.98 |
| | 932 | O | ASP | 131 | 119.762 | -3.837 | 51.341 | 1.00 | 64.40 |
| 40 | 933 | N | GLU | 132 | 119.989 | -5.823 | 52.383 | 1.00 | 70.50 |
| | 934 | CA | GLU | 132 | 118.786 | -6.415 | 51.803 | 1.00 | 72.09 |
| | 935 | CB | GLU | 132 | 118.735 | -7.913 | 52.120 | 1.00 | 78.41 |
| | 936 | CG | GLU | 132 | 119.098 | -8.253 | 53.562 | 1.00 | 92.85 |
| | 937 | CD | GLU | 132 | 117.997 | -8.995 | 54.303 | 1.00 | 100.00 |
| 45 | 938 | OE1 | GLU | 132 | 116.803 | -8.735 | 54.037 | 1.00 | 100.00 |
| | 939 | OE2 | GLU | 132 | 118.331 | -9.837 | 55.165 | 1.00 | 100.00 |
| | 940 | C | GLU | 132 | 117.486 | -5.729 | 52.236 | 1.00 | 69.60 |
| | 941 | O | GLU | 132 | 116.424 | -5.985 | 51.666 | 1.00 | 67.84 |
| | 942 | N | ASN | 133 | 117.575 | -4.849 | 53.230 | 1.00 | 69.95 |
| 50 | 943 | CA | ASN | 133 | 116.408 | -4.124 | 53.726 | 1.00 | 71.81 |

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|----|-----|-----|-----|-----|---------|--------|--------|------|-------|
| | 944 | CB | ASN | 133 | 116.540 | -3.882 | 55.235 | 1.00 | 76.32 |
| | 945 | CG | ASN | 133 | 115.238 | -3.425 | 55.873 | 1.00 | 85.38 |
| | 946 | OD1 | ASN | 133 | 114.202 | -4.076 | 55.731 | 1.00 | 89.18 |
| | 947 | ND2 | ASN | 133 | 115.288 | -2.303 | 56.583 | 1.00 | 85.57 |
| 5 | 948 | C | ASN | 133 | 116.214 | -2.794 | 52.982 | 1.00 | 70.23 |
| | 949 | O | ASN | 133 | 115.184 | -2.132 | 53.136 | 1.00 | 67.90 |
| | 950 | N | GLY | 134 | 117.204 | -2.414 | 52.176 | 1.00 | 67.24 |
| | 951 | CA | GLY | 134 | 117.120 | -1.177 | 51.416 | 1.00 | 63.86 |
| | 952 | C | GLY | 134 | 117.758 | 0.036 | 52.072 | 1.00 | 61.93 |
| 10 | 953 | O | GLY | 134 | 117.712 | 1.138 | 51.520 | 1.00 | 64.71 |
| | 954 | N | LYS | 135 | 118.332 | -0.158 | 53.257 | 1.00 | 57.80 |
| | 955 | CA | LYS | 135 | 118.989 | 0.921 | 53.993 | 1.00 | 52.54 |
| | 956 | CB | LYS | 135 | 118.628 | 0.865 | 55.482 | 1.00 | 54.50 |
| | 957 | CG | LYS | 135 | 117.298 | 1.519 | 55.845 | 1.00 | 58.81 |
| 15 | 958 | CD | LYS | 135 | 116.106 | 0.776 | 55.259 | 1.00 | 65.64 |
| | 959 | CE | LYS | 135 | 114.795 | 1.428 | 55.666 | 1.00 | 66.94 |
| | 960 | NZ | LYS | 135 | 114.629 | 1.450 | 57.145 | 1.00 | 67.92 |
| | 961 | C | LYS | 135 | 120.505 | 0.859 | 53.827 | 1.00 | 46.30 |
| | 962 | O | LYS | 135 | 121.062 | -0.191 | 53.506 | 1.00 | 39.34 |
| 20 | 963 | N | PHE | 136 | 121.168 | 1.988 | 54.058 | 1.00 | 40.70 |
| | 964 | CA | PHE | 136 | 122.619 | 2.066 | 53.929 | 1.00 | 37.70 |
| | 965 | CB | PHE | 136 | 123.082 | 3.525 | 53.941 | 1.00 | 30.32 |
| | 966 | CG | PHE | 136 | 122.848 | 4.238 | 52.644 | 1.00 | 18.97 |
| | 967 | CD1 | PHE | 136 | 121.752 | 5.079 | 52.485 | 1.00 | 16.88 |
| 25 | 968 | CD2 | PHE | 136 | 123.708 | 4.044 | 51.569 | 1.00 | 2.95 |
| | 969 | CE1 | PHE | 136 | 121.512 | 5.714 | 51.269 | 1.00 | 9.36 |
| | 970 | CE2 | PHE | 136 | 123.478 | 4.674 | 50.350 | 1.00 | 8.37 |
| | 971 | CZ | PHE | 136 | 122.376 | 5.510 | 50.200 | 1.00 | 11.64 |
| | 972 | C | PHE | 136 | 123.368 | 1.280 | 54.992 | 1.00 | 40.03 |
| 30 | 973 | O | PHE | 136 | 123.007 | 1.310 | 56.173 | 1.00 | 36.07 |
| | 974 | N | LYS | 137 | 124.404 | 0.564 | 54.554 | 1.00 | 35.20 |
| | 975 | CA | LYS | 137 | 125.232 | -0.232 | 55.451 | 1.00 | 37.62 |
| | 976 | CB | LYS | 137 | 126.333 | -0.957 | 54.670 | 1.00 | 36.07 |
| | 977 | CG | LYS | 137 | 125.845 | -2.039 | 53.721 | 1.00 | 43.95 |
| 35 | 978 | CD | LYS | 137 | 127.016 | -2.672 | 52.985 | 1.00 | 45.68 |
| | 979 | CE | LYS | 137 | 126.558 | -3.745 | 52.011 | 1.00 | 46.97 |
| | 980 | NZ | LYS | 137 | 127.709 | -4.340 | 51.276 | 1.00 | 45.41 |
| | 981 | C | LYS | 137 | 125.872 | 0.698 | 56.472 | 1.00 | 42.74 |
| | 982 | O | LYS | 137 | 126.612 | 1.614 | 56.108 | 1.00 | 49.71 |
| 40 | 983 | N | GLU | 138 | 125.569 | 0.472 | 57.747 | 1.00 | 44.30 |
| | 984 | CA | GLU | 138 | 126.116 | 1.290 | 58.824 | 1.00 | 43.35 |
| | 985 | CB | GLU | 138 | 125.482 | 0.895 | 60.157 | 1.00 | 48.22 |
| | 986 | CG | GLU | 138 | 123.997 | 1.184 | 60.285 | 1.00 | 55.55 |
| | 987 | CD | GLU | 138 | 123.703 | 2.650 | 60.528 | 1.00 | 59.82 |
| 45 | 988 | OE1 | GLU | 138 | 124.127 | 3.180 | 61.577 | 1.00 | 58.06 |
| | 989 | OE2 | GLU | 138 | 123.040 | 3.272 | 59.674 | 1.00 | 70.04 |
| | 990 | C | GLU | 138 | 127.641 | 1.172 | 58.913 | 1.00 | 46.10 |
| | 991 | O | GLU | 138 | 128.283 | 1.909 | 59.662 | 1.00 | 51.05 |
| | 992 | N | SER | 139 | 128.210 | 0.242 | 58.149 | 1.00 | 40.33 |
| 50 | 993 | CA | SER | 139 | 129.653 | 0.027 | 58.122 | 1.00 | 37.26 |

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|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 994 | CB | SER | 139 | 129.975 | -1.354 | 57.541 | 1.00 | 42.99 |
| | 995 | OG | SER | 139 | 129.518 | -1.477 | 56.204 | 1.00 | 42.44 |
| | 996 | C | SER | 139 | 130.384 | 1.114 | 57.326 | 1.00 | 38.83 |
| | 997 | O | SER | 139 | 131.606 | 1.247 | 57.423 | 1.00 | 44.35 |
| 5 | 998 | N | LEU | 140 | 129.633 | 1.875 | 56.531 | 1.00 | 35.64 |
| | 999 | CA | LEU | 140 | 130.191 | 2.960 | 55.721 | 1.00 | 26.87 |
| | 1000 | CB | LEU | 140 | 129.289 | 3.244 | 54.514 | 1.00 | 27.15 |
| | 1001 | CG | LEU | 140 | 129.037 | 2.148 | 53.476 | 1.00 | 27.17 |
| | 1002 | CD1 | LEU | 140 | 127.955 | 2.607 | 52.511 | 1.00 | 23.24 |
| 10 | 1003 | CD2 | LEU | 140 | 130.317 | 1.814 | 52.726 | 1.00 | 21.35 |
| | 1004 | C | LEU | 140 | 130.325 | 4.241 | 56.547 | 1.00 | 23.48 |
| | 1005 | O | LEU | 140 | 130.817 | 5.254 | 56.054 | 1.00 | 18.12 |
| | 1006 | N | ALA | 141 | 129.883 | 4.178 | 57.803 | 1.00 | 21.14 |
| | 1007 | CA | ALA | 141 | 129.916 | 5.311 | 58.725 | 1.00 | 23.07 |
| 15 | 1008 | CB | ALA | 141 | 129.182 | 4.951 | 60.007 | 1.00 | 13.93 |
| | 1009 | C | ALA | 141 | 131.316 | 5.829 | 59.053 | 1.00 | 29.68 |
| | 1010 | O | ALA | 141 | 131.465 | 6.917 | 59.614 | 1.00 | 34.02 |
| | 1011 | N | SER | 142 | 132.334 | 5.045 | 58.710 | 1.00 | 31.98 |
| | 1012 | CA | SER | 142 | 133.723 | 5.413 | 58.963 | 1.00 | 25.78 |
| 20 | 1013 | CB | SER | 142 | 134.482 | 4.211 | 59.534 | 1.00 | 27.76 |
| | 1014 | OG | SER | 142 | 134.293 | 3.059 | 58.731 | 1.00 | 23.34 |
| | 1015 | C | SER | 142 | 134.436 | 5.957 | 57.719 | 1.00 | 26.37 |
| | 1016 | O | SER | 142 | 135.629 | 6.255 | 57.761 | 1.00 | 36.05 |
| | 1017 | N | ASP | 143 | 133.699 | 6.078 | 56.617 | 1.00 | 19.43 |
| 25 | 1018 | CA | ASP | 143 | 134.237 | 6.596 | 55.361 | 1.00 | 13.45 |
| | 1019 | CB | ASP | 143 | 133.794 | 5.701 | 54.194 | 1.00 | 12.41 |
| | 1020 | CG | ASP | 143 | 134.284 | 6.196 | 52.835 | 1.00 | 22.67 |
| | 1021 | OD1 | ASP | 143 | 133.710 | 5.759 | 51.811 | 1.00 | 21.93 |
| | 1022 | OD2 | ASP | 143 | 135.239 | 7.004 | 52.778 | 1.00 | 35.17 |
| 30 | 1023 | C | ASP | 143 | 133.727 | 8.025 | 55.162 | 1.00 | 19.69 |
| | 1024 | O | ASP | 143 | 132.675 | 8.238 | 54.559 | 1.00 | 21.70 |
| | 1025 | N | VAL | 144 | 134.485 | 8.997 | 55.664 | 1.00 | 21.88 |
| | 1026 | CA | VAL | 144 | 134.120 | 10.411 | 55.566 | 1.00 | 19.30 |
| | 1027 | CB | VAL | 144 | 135.093 | 11.295 | 56.376 | 1.00 | 16.67 |
| 35 | 1028 | CG1 | VAL | 144 | 134.789 | 12.769 | 56.155 | 1.00 | 22.12 |
| | 1029 | CG2 | VAL | 144 | 134.978 | 10.961 | 57.857 | 1.00 | 20.43 |
| | 1030 | C | VAL | 144 | 133.997 | 10.942 | 54.136 | 1.00 | 18.93 |
| | 1031 | O | VAL | 144 | 133.012 | 11.603 | 53.801 | 1.00 | 23.53 |
| | 1032 | N | LEU | 145 | 134.984 | 10.657 | 53.293 | 1.00 | 15.19 |
| 40 | 1033 | CA | LEU | 145 | 134.940 | 11.122 | 51.912 | 1.00 | 18.54 |
| | 1034 | CB | LEU | 145 | 136.238 | 10.780 | 51.181 | 1.00 | 22.93 |
| | 1035 | CG | LEU | 145 | 137.524 | 11.410 | 51.722 | 1.00 | 23.25 |
| | 1036 | CD1 | LEU | 145 | 138.647 | 11.189 | 50.715 | 1.00 | 24.40 |
| | 1037 | CD2 | LEU | 145 | 137.327 | 12.898 | 51.968 | 1.00 | 18.75 |
| 45 | 1038 | C | LEU | 145 | 133.744 | 10.535 | 51.168 | 1.00 | 23.90 |
| | 1039 | O | LEU | 145 | 133.236 | 11.135 | 50.219 | 1.00 | 26.81 |
| | 1040 | N | GLY | 146 | 133.303 | 9.358 | 51.610 | 1.00 | 24.92 |
| | 1041 | CA | GLY | 146 | 132.159 | 8.705 | 50.999 | 1.00 | 21.44 |
| | 1042 | C | GLY | 146 | 130.868 | 9.313 | 51.512 | 1.00 | 19.58 |
| 50 | 1043 | O | GLY | 146 | 129.953 | 9.591 | 50.740 | 1.00 | 22.50 |

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|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 1044 | N | LEU | 147 | 130.805 | 9.524 | 52.823 | 1.00 | 9.20 |
| | 1045 | CA | LEU | 147 | 129.643 | 10.116 | 53.467 | 1.00 | 7.33 |
| | 1046 | CB | LEU | 147 | 129.849 | 10.163 | 54.980 | 1.00 | 7.87 |
| | 1047 | CG | LEU | 147 | 129.927 | 8.831 | 55.721 | 1.00 | 12.02 |
| 5 | 1048 | CD1 | LEU | 147 | 130.341 | 9.066 | 57.157 | 1.00 | 8.20 |
| | 1049 | CD2 | LEU | 147 | 128.583 | 8.122 | 55.656 | 1.00 | 15.08 |
| | 1050 | C | LEU | 147 | 129.388 | 11.527 | 52.945 | 1.00 | 20.24 |
| | 1051 | O | LEU | 147 | 128.244 | 11.900 | 52.680 | 1.00 | 27.36 |
| | 1052 | N | LEU | 148 | 130.462 | 12.303 | 52.795 | 1.00 | 20.47 |
| 10 | 1053 | CA | LEU | 148 | 130.371 | 13.676 | 52.304 | 1.00 | 20.11 |
| | 1054 | CB | LEU | 148 | 131.751 | 14.347 | 52.330 | 1.00 | 16.79 |
| | 1055 | CG | LEU | 148 | 131.829 | 15.805 | 51.857 | 1.00 | 13.41 |
| | 1056 | CD1 | LEU | 148 | 130.897 | 16.683 | 52.683 | 1.00 | 6.32 |
| | 1057 | CD2 | LEU | 148 | 133.256 | 16.306 | 51.961 | 1.00 | 9.98 |
| 15 | 1058 | C | LEU | 148 | 129.777 | 13.758 | 50.895 | 1.00 | 16.22 |
| | 1059 | O | LEU | 148 | 128.838 | 14.520 | 50.657 | 1.00 | 19.05 |
| | 1060 | N | ASN | 149 | 130.332 | 12.985 | 49.965 | 1.00 | 14.19 |
| | 1061 | CA | ASN | 149 | 129.840 | 12.986 | 48.592 | 1.00 | 19.68 |
| | 1062 | CB | ASN | 149 | 130.776 | 12.199 | 47.678 | 1.00 | 17.57 |
| 20 | 1063 | CG | ASN | 149 | 132.009 | 12.987 | 47.306 | 1.00 | 21.68 |
| | 1064 | OD1 | ASN | 149 | 132.904 | 13.181 | 48.129 | 1.00 | 27.23 |
| | 1065 | ND2 | ASN | 149 | 132.055 | 13.469 | 46.067 | 1.00 | 17.93 |
| | 1066 | C | ASN | 149 | 128.414 | 12.461 | 48.486 | 1.00 | 24.02 |
| | 1067 | O | ASN | 149 | 127.676 | 12.829 | 47.571 | 1.00 | 25.30 |
| 25 | 1068 | N | LEU | 150 | 128.033 | 11.596 | 49.424 | 1.00 | 23.15 |
| | 1069 | CA | LEU | 150 | 126.685 | 11.049 | 49.449 | 1.00 | 19.85 |
| | 1070 | CB | LEU | 150 | 126.606 | 9.844 | 50.391 | 1.00 | 15.00 |
| | 1071 | CG | LEU | 150 | 125.224 | 9.198 | 50.548 | 1.00 | 14.74 |
| | 1072 | CD1 | LEU | 150 | 124.735 | 8.634 | 49.215 | 1.00 | 8.02 |
| 30 | 1073 | CD2 | LEU | 150 | 125.287 | 8.115 | 51.600 | 1.00 | 2.00 |
| | 1074 | C | LEU | 150 | 125.745 | 12.153 | 49.925 | 1.00 | 20.18 |
| | 1075 | O | LEU | 150 | 124.640 | 12.304 | 49.404 | 1.00 | 22.47 |
| | 1076 | N | TYR | 151 | 126.209 | 12.930 | 50.904 | 1.00 | 18.20 |
| | 1077 | CA | TYR | 151 | 125.440 | 14.041 | 51.455 | 1.00 | 18.43 |
| 35 | 1078 | CB | TYR | 151 | 126.226 | 14.739 | 52.569 | 1.00 | 10.57 |
| | 1079 | CG | TYR | 151 | 125.598 | 16.032 | 53.044 | 1.00 | 11.49 |
| | 1080 | CD1 | TYR | 151 | 124.759 | 16.056 | 54.156 | 1.00 | 5.47 |
| | 1081 | CE1 | TYR | 151 | 124.171 | 17.242 | 54.586 | 1.00 | 8.73 |
| | 1082 | CD2 | TYR | 151 | 125.835 | 17.234 | 52.372 | 1.00 | 10.72 |
| 40 | 1083 | CE2 | TYR | 151 | 125.250 | 18.421 | 52.791 | 1.00 | 9.08 |
| | 1084 | CZ | TYR | 151 | 124.421 | 18.420 | 53.898 | 1.00 | 11.39 |
| | 1085 | OH | TYR | 151 | 123.845 | 19.598 | 54.316 | 1.00 | 11.19 |
| | 1086 | C | TYR | 151 | 125.117 | 15.041 | 50.355 | 1.00 | 17.39 |
| | 1087 | O | TYR | 151 | 123.990 | 15.521 | 50.256 | 1.00 | 26.93 |
| 45 | 1088 | N | GLU | 152 | 126.121 | 15.374 | 49.552 | 1.00 | 15.23 |
| | 1089 | CA | GLU | 152 | 125.937 | 16.316 | 48.455 | 1.00 | 18.45 |
| | 1090 | CB | GLU | 152 | 127.282 | 16.649 | 47.798 | 1.00 | 14.61 |
| | 1091 | CG | GLU | 152 | 128.316 | 17.293 | 48.727 | 1.00 | 17.73 |
| | 1092 | CD | GLU | 152 | 127.962 | 18.712 | 49.169 | 1.00 | 16.74 |
| 50 | 1093 | OE1 | GLU | 152 | 126.980 | 19.292 | 48.662 | 1.00 | 16.63 |

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|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 1094 | OE2 | GLU | 152 | 128.681 | 19.252 | 50.034 | 1.00 | 22.78 |
| | 1095 | C | GLU | 152 | 124.977 | 15.750 | 47.413 | 1.00 | 13.63 |
| | 1096 | O | GLU | 152 | 124.114 | 16.463 | 46.904 | 1.00 | 20.19 |
| | 1097 | N | ALA | 153 | 125.115 | 14.458 | 47.125 | 1.00 | 18.04 |
| 5 | 1098 | CA | ALA | 153 | 124.271 | 13.778 | 46.143 | 1.00 | 14.37 |
| | 1099 | CB | ALA | 153 | 124.859 | 12.417 | 45.794 | 1.00 | 13.44 |
| | 1100 | C | ALA | 153 | 122.815 | 13.624 | 46.580 | 1.00 | 13.36 |
| | 1101 | O | ALA | 153 | 121.921 | 13.577 | 45.738 | 1.00 | 11.20 |
| | 1102 | N | SER | 154 | 122.574 | 13.568 | 47.889 | 1.00 | 16.02 |
| 10 | 1103 | CA | SER | 154 | 121.218 | 13.413 | 48.416 | 1.00 | 13.22 |
| | 1104 | CB | SER | 154 | 121.250 | 13.157 | 49.928 | 1.00 | 8.73 |
| | 1105 | OG | SER | 154 | 121.581 | 14.330 | 50.651 | 1.00 | 16.49 |
| | 1106 | C | SER | 154 | 120.312 | 14.607 | 48.118 | 1.00 | 14.26 |
| | 1107 | O | SER | 154 | 119.087 | 14.504 | 48.207 | 1.00 | 26.54 |
| 15 | 1108 | N | HIS | 155 | 120.915 | 15.735 | 47.757 | 1.00 | 14.00 |
| | 1109 | CA | HIS | 155 | 120.154 | 16.942 | 47.457 | 1.00 | 8.22 |
| | 1110 | CB | HIS | 155 | 120.920 | 18.177 | 47.928 | 1.00 | 2.00 |
| | 1111 | CG | HIS | 155 | 120.932 | 18.340 | 49.415 | 1.00 | 2.00 |
| | 1112 | CD2 | HIS | 155 | 120.036 | 18.914 | 50.255 | 1.00 | 3.97 |
| 20 | 1113 | ND1 | HIS | 155 | 121.946 | 17.856 | 50.211 | 1.00 | 3.74 |
| | 1114 | CE1 | HIS | 155 | 121.676 | 18.123 | 51.476 | 1.00 | 12.80 |
| | 1115 | NE2 | HIS | 155 | 120.522 | 18.764 | 51.529 | 1.00 | 11.17 |
| | 1116 | C | HIS | 155 | 119.742 | 17.092 | 45.997 | 1.00 | 10.18 |
| | 1117 | O | HIS | 155 | 119.025 | 18.030 | 45.645 | 1.00 | 16.07 |
| 25 | 1118 | N | VAL | 156 | 120.182 | 16.163 | 45.152 | 1.00 | 6.86 |
| | 1119 | CA | VAL | 156 | 119.843 | 16.202 | 43.733 | 1.00 | 7.09 |
| | 1120 | CB | VAL | 156 | 121.109 | 16.099 | 42.823 | 1.00 | 5.97 |
| | 1121 | CG1 | VAL | 156 | 122.161 | 17.113 | 43.248 | 1.00 | 2.00 |
| | 1122 | CG2 | VAL | 156 | 121.678 | 14.682 | 42.841 | 1.00 | 4.04 |
| 30 | 1123 | C | VAL | 156 | 118.866 | 15.087 | 43.354 | 1.00 | 11.84 |
| | 1124 | O | VAL | 156 | 118.644 | 14.827 | 42.170 | 1.00 | 13.76 |
| | 1125 | N | ARG | 157 | 118.264 | 14.443 | 44.351 | 1.00 | 12.59 |
| | 1126 | CA | ARG | 157 | 117.329 | 13.357 | 44.074 | 1.00 | 21.43 |
| | 1127 | CB | ARG | 157 | 117.224 | 12.398 | 45.271 | 1.00 | 17.56 |
| 35 | 1128 | CG | ARG | 157 | 116.482 | 12.908 | 46.491 | 1.00 | 22.45 |
| | 1129 | CD | ARG | 157 | 116.525 | 11.846 | 47.583 | 1.00 | 26.00 |
| | 1130 | NE | ARG | 157 | 115.512 | 12.037 | 48.620 | 1.00 | 35.19 |
| | 1131 | CZ | ARG | 157 | 114.360 | 11.370 | 48.676 | 1.00 | 40.41 |
| | 1132 | NH1 | ARG | 157 | 114.064 | 10.465 | 47.753 | 1.00 | 42.25 |
| 40 | 1133 | NH2 | ARG | 157 | 113.505 | 11.598 | 49.664 | 1.00 | 42.66 |
| | 1134 | C | ARG | 157 | 115.945 | 13.815 | 43.609 | 1.00 | 22.46 |
| | 1135 | O | ARG | 157 | 115.473 | 14.885 | 43.985 | 1.00 | 28.62 |
| | 1136 | N | THR | 158 | 115.334 | 13.012 | 42.740 | 1.00 | 30.57 |
| | 1137 | CA | THR | 158 | 114.003 | 13.287 | 42.200 | 1.00 | 23.48 |
| 45 | 1138 | CB | THR | 158 | 113.951 | 13.012 | 40.675 | 1.00 | 18.85 |
| | 1139 | OG1 | THR | 158 | 114.132 | 11.613 | 40.424 | 1.00 | 23.14 |
| | 1140 | CG2 | THR | 158 | 115.044 | 13.781 | 39.959 | 1.00 | 5.29 |
| | 1141 | C | THR | 158 | 112.962 | 12.409 | 42.911 | 1.00 | 26.07 |
| | 1142 | O | THR | 158 | 113.258 | 11.786 | 43.936 | 1.00 | 29.73 |
| 50 | 1143 | N | HIS | 159 | 111.745 | 12.362 | 42.373 | 1.00 | 25.85 |

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|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 1144 | CA | HIS | 159 | 110.681 | 11.551 | 42.967 | 1.00 | 24.71 |
| | 1145 | CB | HIS | 159 | 109.312 | 11.987 | 42.435 | 1.00 | 24.02 |
| | 1146 | CG | HIS | 159 | 108.903 | 13.358 | 42.872 | 1.00 | 20.05 |
| | 1147 | CD2 | HIS | 159 | 108.888 | 14.538 | 42.209 | 1.00 | 14.66 |
| 5 | 1148 | ND1 | HIS | 159 | 108.453 | 13.629 | 44.147 | 1.00 | 22.06 |
| | 1149 | CE1 | HIS | 159 | 108.179 | 14.917 | 44.250 | 1.00 | 20.70 |
| | 1150 | NE2 | HIS | 159 | 108.434 | 15.492 | 43.088 | 1.00 | 18.69 |
| | 1151 | C | HIS | 159 | 110.893 | 10.054 | 42.723 | 1.00 | 28.82 |
| | 1152 | O | HIS | 159 | 110.377 | 9.211 | 43.464 | 1.00 | 29.90 |
| 10 | 1153 | N | ALA | 160 | 111.674 | 9.733 | 41.695 | 1.00 | 22.36 |
| | 1154 | CA | ALA | 160 | 111.966 | 8.351 | 41.341 | 1.00 | 16.69 |
| | 1155 | CB | ALA | 160 | 112.118 | 8.233 | 39.835 | 1.00 | 12.78 |
| | 1156 | C | ALA | 160 | 113.218 | 7.821 | 42.038 | 1.00 | 24.25 |
| | 1157 | O | ALA | 160 | 113.748 | 6.775 | 41.655 | 1.00 | 30.58 |
| 15 | 1158 | N | ASP | 161 | 113.679 | 8.531 | 43.066 | 1.00 | 27.69 |
| | 1159 | CA | ASP | 161 | 114.880 | 8.134 | 43.800 | 1.00 | 24.25 |
| | 1160 | CB | ASP | 161 | 115.968 | 9.212 | 43.669 | 1.00 | 22.91 |
| | 1161 | CG | ASP | 161 | 116.356 | 9.495 | 42.222 | 1.00 | 29.35 |
| | 1162 | OD1 | ASP | 161 | 116.405 | 8.550 | 41.404 | 1.00 | 29.54 |
| 20 | 1163 | OD2 | ASP | 161 | 116.623 | 10.672 | 41.906 | 1.00 | 19.16 |
| | 1164 | C | ASP | 161 | 114.626 | 7.840 | 45.281 | 1.00 | 26.01 |
| | 1165 | O | ASP | 161 | 115.308 | 8.380 | 46.154 | 1.00 | 34.22 |
| | 1166 | N | ASP | 162 | 113.670 | 6.957 | 45.561 | 1.00 | 28.71 |
| | 1167 | CA | ASP | 162 | 113.339 | 6.590 | 46.939 | 1.00 | 28.70 |
| 25 | 1168 | CB | ASP | 162 | 111.999 | 5.859 | 46.993 | 1.00 | 34.90 |
| | 1169 | CG | ASP | 162 | 110.851 | 6.726 | 46.536 | 1.00 | 42.80 |
| | 1170 | OD1 | ASP | 162 | 110.426 | 7.600 | 47.322 | 1.00 | 36.44 |
| | 1171 | OD2 | ASP | 162 | 110.386 | 6.543 | 45.389 | 1.00 | 43.54 |
| | 1172 | C | ASP | 162 | 114.423 | 5.728 | 47.573 | 1.00 | 27.14 |
| 30 | 1173 | O | ASP | 162 | 114.386 | 5.441 | 48.769 | 1.00 | 28.39 |
| | 1174 | N | ILE | 163 | 115.378 | 5.302 | 46.756 | 1.00 | 26.67 |
| | 1175 | CA | ILE | 163 | 116.485 | 4.486 | 47.229 | 1.00 | 27.39 |
| | 1176 | CB | ILE | 163 | 117.250 | 3.866 | 46.030 | 1.00 | 24.84 |
| | 1177 | CG2 | ILE | 163 | 118.201 | 4.881 | 45.412 | 1.00 | 29.37 |
| 35 | 1178 | CG1 | ILE | 163 | 118.015 | 2.623 | 46.471 | 1.00 | 30.57 |
| | 1179 | CD1 | ILE | 163 | 118.639 | 1.863 | 45.323 | 1.00 | 43.90 |
| | 1180 | C | ILE | 163 | 117.407 | 5.372 | 48.078 | 1.00 | 28.12 |
| | 1181 | O | ILE | 163 | 118.169 | 4.881 | 48.912 | 1.00 | 29.38 |
| | 1182 | N | LEU | 164 | 117.277 | 6.686 | 47.890 | 1.00 | 30.46 |
| 40 | 1183 | CA | LEU | 164 | 118.070 | 7.684 | 48.607 | 1.00 | 24.33 |
| | 1184 | CB | LEU | 164 | 118.646 | 8.695 | 47.612 | 1.00 | 16.04 |
| | 1185 | CG | LEU | 164 | 119.602 | 8.181 | 46.538 | 1.00 | 20.33 |
| | 1186 | CD1 | LEU | 164 | 119.864 | 9.271 | 45.514 | 1.00 | 22.74 |
| | 1187 | CD2 | LEU | 164 | 120.894 | 7.720 | 47.184 | 1.00 | 17.92 |
| 45 | 1188 | C | LEU | 164 | 117.259 | 8.441 | 49.658 | 1.00 | 23.88 |
| | 1189 | O | LEU | 164 | 117.667 | 9.518 | 50.101 | 1.00 | 32.16 |
| | 1190 | N | GLU | 165 | 116.120 | 7.882 | 50.061 | 1.00 | 21.56 |
| | 1191 | CA | GLU | 165 | 115.256 | 8.529 | 51.043 | 1.00 | 18.89 |
| | 1192 | CB | GLU | 165 | 113.947 | 7.755 | 51.202 | 1.00 | 24.79 |
| 50 | 1193 | CG | GLU | 165 | 114.127 | 6.324 | 51.689 | 1.00 | 48.18 |

| | | | | | | | | | |
|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 1194 | CD | GLU | 165 | 112.819 | 5.561 | 51.814 | 1.00 | 57.24 |
| | 1195 | OE1 | GLU | 165 | 111.765 | 6.076 | 51.375 | 1.00 | 63.77 |
| | 1196 | OE2 | GLU | 165 | 112.850 | 4.434 | 52.353 | 1.00 | 62.32 |
| 5 | 1197 | C | GLU | 165 | 115.907 | 8.727 | 52.405 | 1.00 | 16.81 |
| | 1198 | O | GLU | 165 | 115.598 | 9.687 | 53.106 | 1.00 | 18.04 |
| | 1199 | N | ASP | 166 | 116.817 | 7.828 | 52.771 | 1.00 | 23.03 |
| | 1200 | CA | ASP | 166 | 117.497 | 7.914 | 54.061 | 1.00 | 27.94 |
| | 1201 | CB | ASP | 166 | 117.383 | 6.579 | 54.811 | 1.00 | 35.23 |
| 10 | 1202 | CG | ASP | 166 | 115.936 | 6.177 | 55.082 | 1.00 | 50.03 |
| | 1203 | OD1 | ASP | 166 | 115.565 | 5.024 | 54.771 | 1.00 | 57.17 |
| | 1204 | OD2 | ASP | 166 | 115.169 | 7.013 | 55.606 | 1.00 | 53.93 |
| | 1205 | C | ASP | 166 | 118.966 | 8.330 | 53.943 | 1.00 | 24.13 |
| | 1206 | O | ASP | 166 | 119.674 | 8.409 | 54.950 | 1.00 | 23.24 |
| 15 | 1207 | N | ALA | 167 | 119.401 | 8.638 | 52.721 | 1.00 | 14.78 |
| | 1208 | CA | ALA | 167 | 120.780 | 9.044 | 52.443 | 1.00 | 16.72 |
| | 1209 | CB | ALA | 167 | 120.993 | 9.169 | 50.948 | 1.00 | 12.70 |
| | 1210 | C | ALA | 167 | 121.215 | 10.333 | 53.136 | 1.00 | 24.13 |
| | 1211 | O | ALA | 167 | 122.355 | 10.443 | 53.590 | 1.00 | 29.67 |
| 20 | 1212 | N | LEU | 168 | 120.317 | 11.313 | 53.193 | 1.00 | 27.80 |
| | 1213 | CA | LEU | 168 | 120.614 | 12.590 | 53.831 | 1.00 | 19.27 |
| | 1214 | CB | LEU | 168 | 119.540 | 13.623 | 53.487 | 1.00 | 23.80 |
| | 1215 | CG | LEU | 168 | 119.706 | 15.016 | 54.099 | 1.00 | 18.12 |
| | 1216 | CD1 | LEU | 168 | 121.006 | 15.642 | 53.626 | 1.00 | 19.21 |
| 25 | 1217 | CD2 | LEU | 168 | 118.524 | 15.890 | 53.719 | 1.00 | 17.36 |
| | 1218 | C | LEU | 168 | 120.730 | 12.450 | 55.343 | 1.00 | 20.39 |
| | 1219 | O | LEU | 168 | 121.663 | 12.973 | 55.943 | 1.00 | 26.94 |
| | 1220 | N | ALA | 169 | 119.776 | 11.755 | 55.954 | 1.00 | 22.95 |
| | 1221 | CA | ALA | 169 | 119.784 | 11.555 | 57.400 | 1.00 | 28.99 |
| 30 | 1222 | CB | ALA | 169 | 118.472 | 10.934 | 57.856 | 1.00 | 26.34 |
| | 1223 | C | ALA | 169 | 120.959 | 10.676 | 57.816 | 1.00 | 31.11 |
| | 1224 | O | ALA | 169 | 121.529 | 10.855 | 58.895 | 1.00 | 32.24 |
| | 1225 | N | PHE | 170 | 121.319 | 9.736 | 56.944 | 1.00 | 26.27 |
| | 1226 | CA | PHE | 170 | 122.423 | 8.819 | 57.197 | 1.00 | 22.01 |
| 35 | 1227 | CB | PHE | 170 | 122.448 | 7.714 | 56.135 | 1.00 | 20.64 |
| | 1228 | CG | PHE | 170 | 123.592 | 6.747 | 56.284 | 1.00 | 28.63 |
| | 1229 | CD1 | PHE | 170 | 123.622 | 5.837 | 57.338 | 1.00 | 28.29 |
| | 1230 | CD2 | PHE | 170 | 124.642 | 6.745 | 55.368 | 1.00 | 25.46 |
| | 1231 | CE1 | PHE | 170 | 124.683 | 4.938 | 57.479 | 1.00 | 27.46 |
| 40 | 1232 | CE2 | PHE | 170 | 125.706 | 5.850 | 55.500 | 1.00 | 24.24 |
| | 1233 | CZ | PHE | 170 | 125.726 | 4.945 | 56.558 | 1.00 | 22.35 |
| | 1234 | C | PHE | 170 | 123.752 | 9.564 | 57.205 | 1.00 | 20.63 |
| | 1235 | O | PHE | 170 | 124.440 | 9.610 | 58.224 | 1.00 | 23.76 |
| | 1236 | N | SER | 171 | 124.095 | 10.156 | 56.066 | 1.00 | 16.15 |
| 45 | 1237 | CA | SER | 171 | 125.340 | 10.899 | 55.918 | 1.00 | 12.93 |
| | 1238 | CB | SER | 171 | 125.476 | 11.429 | 54.488 | 1.00 | 12.97 |
| | 1239 | OG | SER | 171 | 124.397 | 12.281 | 54.152 | 1.00 | 12.50 |
| | 1240 | C | SER | 171 | 125.479 | 12.047 | 56.912 | 1.00 | 13.92 |
| | 1241 | O | SER | 171 | 126.567 | 12.297 | 57.420 | 1.00 | 15.50 |
| 50 | 1242 | N | THR | 172 | 124.372 | 12.726 | 57.205 | 1.00 | 16.38 |
| | 1243 | CA | THR | 172 | 124.383 | 13.854 | 58.137 | 1.00 | 16.69 |

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|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 1244 | CB | THR | 172 | 123.000 | 14.564 | 58.196 | 1.00 | 14.70 |
| | 1245 | OG1 | THR | 172 | 122.758 | 15.259 | 56.966 | 1.00 | 12.00 |
| | 1246 | CG2 | THR | 172 | 122.946 | 15.559 | 59.348 | 1.00 | 6.76 |
| 5 | 1247 | C | THR | 172 | 124.813 | 13.486 | 59.556 | 1.00 | 19.18 |
| | 1248 | O | THR | 172 | 125.759 | 14.067 | 60.086 | 1.00 | 22.93 |
| | 1249 | N | ILE | 173 | 124.129 | 12.516 | 60.160 | 1.00 | 22.35 |
| | 1250 | CA | ILE | 173 | 124.439 | 12.112 | 61.529 | 1.00 | 26.29 |
| | 1251 | CB | ILE | 173 | 123.428 | 11.061 | 62.070 | 1.00 | 29.19 |
| 10 | 1252 | CG2 | ILE | 173 | 123.553 | 9.747 | 61.305 | 1.00 | 26.89 |
| | 1253 | CG1 | ILE | 173 | 123.657 | 10.844 | 63.572 | 1.00 | 34.59 |
| | 1254 | CD1 | ILE | 173 | 122.655 | 9.928 | 64.240 | 1.00 | 35.92 |
| | 1255 | C | ILE | 173 | 125.868 | 11.602 | 61.702 | 1.00 | 27.07 |
| | 1256 | O | ILE | 173 | 126.481 | 11.801 | 62.754 | 1.00 | 30.04 |
| 15 | 1257 | N | HIS | 174 | 126.404 | 10.972 | 60.662 | 1.00 | 18.99 |
| | 1258 | CA | HIS | 174 | 127.757 | 10.441 | 60.721 | 1.00 | 26.30 |
| | 1259 | CB | HIS | 174 | 127.895 | 9.228 | 59.799 | 1.00 | 36.54 |
| | 1260 | CG | HIS | 174 | 127.114 | 8.034 | 60.257 | 1.00 | 41.37 |
| | 1261 | CD2 | HIS | 174 | 126.355 | 7.147 | 59.571 | 1.00 | 35.65 |
| 20 | 1262 | ND1 | HIS | 174 | 127.057 | 7.644 | 61.579 | 1.00 | 39.38 |
| | 1263 | CE1 | HIS | 174 | 126.295 | 6.569 | 61.687 | 1.00 | 33.20 |
| | 1264 | NE2 | HIS | 174 | 125.857 | 6.248 | 60.483 | 1.00 | 35.00 |
| | 1265 | C | HIS | 174 | 128.804 | 11.504 | 60.407 | 1.00 | 27.93 |
| | 1266 | O | HIS | 174 | 129.945 | 11.419 | 60.872 | 1.00 | 25.80 |
| 25 | 1267 | N | LEU | 175 | 128.410 | 12.508 | 59.626 | 1.00 | 25.88 |
| | 1268 | CA | LEU | 175 | 129.312 | 13.600 | 59.280 | 1.00 | 17.20 |
| | 1269 | CB | LEU | 175 | 128.804 | 14.376 | 58.066 | 1.00 | 12.92 |
| | 1270 | CG | LEU | 175 | 129.069 | 13.747 | 56.696 | 1.00 | 4.37 |
| | 1271 | CD1 | LEU | 175 | 128.472 | 14.624 | 55.606 | 1.00 | 2.00 |
| 30 | 1272 | CD2 | LEU | 175 | 130.566 | 13.572 | 56.482 | 1.00 | 6.69 |
| | 1273 | C | LEU | 175 | 129.459 | 14.530 | 60.470 | 1.00 | 17.96 |
| | 1274 | O | LEU | 175 | 130.534 | 15.074 | 60.705 | 1.00 | 30.10 |
| | 1275 | N | GLU | 176 | 128.375 | 14.699 | 61.225 | 1.00 | 17.67 |
| | 1276 | CA | GLU | 176 | 128.386 | 15.550 | 62.412 | 1.00 | 27.17 |
| 35 | 1277 | CB | GLU | 176 | 126.969 | 15.740 | 62.959 | 1.00 | 26.19 |
| | 1278 | CG | GLU | 176 | 125.997 | 16.452 | 62.037 | 1.00 | 39.91 |
| | 1279 | CD | GLU | 176 | 124.606 | 16.584 | 62.645 | 1.00 | 51.08 |
| | 1280 | OE1 | GLU | 176 | 124.184 | 15.676 | 63.398 | 1.00 | 49.19 |
| | 1281 | OE2 | GLU | 176 | 123.932 | 17.600 | 62.368 | 1.00 | 52.29 |
| 40 | 1282 | C | GLU | 176 | 129.241 | 14.913 | 63.505 | 1.00 | 29.58 |
| | 1283 | O | GLU | 176 | 129.953 | 15.604 | 64.237 | 1.00 | 37.29 |
| | 1284 | N | SER | 177 | 129.156 | 13.589 | 63.604 | 1.00 | 31.69 |
| | 1285 | CA | SER | 177 | 129.883 | 12.816 | 64.607 | 1.00 | 28.71 |
| | 1286 | CB | SER | 177 | 129.310 | 11.395 | 64.678 | 1.00 | 24.94 |
| 45 | 1287 | OG | SER | 177 | 129.868 | 10.660 | 65.755 | 1.00 | 27.40 |
| | 1288 | C | SER | 177 | 131.392 | 12.758 | 64.370 | 1.00 | 25.55 |
| | 1289 | O | SER | 177 | 132.177 | 12.795 | 65.324 | 1.00 | 17.66 |
| | 1290 | N | ALA | 178 | 131.787 | 12.682 | 63.102 | 1.00 | 17.70 |
| | 1291 | CA | ALA | 178 | 133.195 | 12.600 | 62.723 | 1.00 | 19.27 |
| 50 | 1292 | CB | ALA | 178 | 133.330 | 11.789 | 61.441 | 1.00 | 22.41 |
| | 1293 | C | ALA | 178 | 133.897 | 13.948 | 62.558 | 1.00 | 24.31 |

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|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 1294 | O | ALA | 178 | 135.107 | 14.054 | 62.769 | 1.00 | 24.74 |
| | 1295 | N | ALA | 179 | 133.124 | 14.975 | 62.214 | 1.00 | 25.32 |
| | 1296 | CA | ALA | 179 | 133.630 | 16.326 | 61.971 | 1.00 | 25.36 |
| | 1297 | CB | ALA | 179 | 132.460 | 17.289 | 61.779 | 1.00 | 32.63 |
| 5 | 1298 | C | ALA | 179 | 134.658 | 16.943 | 62.928 | 1.00 | 23.67 |
| | 1299 | O | ALA | 179 | 135.706 | 17.420 | 62.487 | 1.00 | 23.47 |
| | 1300 | N | PRO | 180 | 134.384 | 16.929 | 64.244 | 1.00 | 21.48 |
| | 1301 | CD | PRO | 180 | 133.196 | 16.355 | 64.900 | 1.00 | 20.79 |
| 10 | 1302 | CA | PRO | 180 | 135.291 | 17.505 | 65.247 | 1.00 | 20.21 |
| | 1303 | CB | PRO | 180 | 134.601 | 17.155 | 66.568 | 1.00 | 10.68 |
| | 1304 | CG | PRO | 180 | 133.162 | 17.108 | 66.203 | 1.00 | 16.34 |
| | 1305 | C | PRO | 180 | 136.747 | 17.040 | 65.264 | 1.00 | 21.05 |
| | 1306 | O | PRO | 180 | 137.623 | 17.772 | 65.722 | 1.00 | 30.38 |
| 15 | 1307 | N | HIS | 181 | 137.015 | 15.846 | 64.750 | 1.00 | 24.41 |
| | 1308 | CA | HIS | 181 | 138.372 | 15.310 | 64.785 | 1.00 | 20.38 |
| | 1309 | CB | HIS | 181 | 138.359 | 13.955 | 65.498 | 1.00 | 22.19 |
| | 1310 | CG | HIS | 181 | 137.686 | 13.989 | 66.837 | 1.00 | 20.19 |
| | 1311 | CD2 | HIS | 181 | 138.077 | 14.524 | 68.018 | 1.00 | 22.10 |
| 20 | 1312 | ND1 | HIS | 181 | 136.437 | 13.448 | 67.055 | 1.00 | 24.79 |
| | 1313 | CE1 | HIS | 181 | 136.086 | 13.649 | 68.313 | 1.00 | 28.39 |
| | 1314 | NE2 | HIS | 181 | 137.064 | 14.300 | 68.919 | 1.00 | 34.90 |
| | 1315 | C | HIS | 181 | 139.073 | 15.184 | 63.443 | 1.00 | 16.56 |
| | 1316 | O | HIS | 181 | 140.138 | 14.575 | 63.351 | 1.00 | 20.78 |
| 25 | 1317 | N | LEU | 182 | 138.496 | 15.775 | 62.407 | 1.00 | 19.38 |
| | 1318 | CA | LEU | 182 | 139.095 | 15.698 | 61.082 | 1.00 | 19.81 |
| | 1319 | CB | LEU | 182 | 138.023 | 15.838 | 59.999 | 1.00 | 12.64 |
| | 1320 | CG | LEU | 182 | 136.883 | 14.822 | 60.017 | 1.00 | 9.36 |
| | 1321 | CD1 | LEU | 182 | 135.883 | 15.191 | 58.946 | 1.00 | 6.26 |
| 30 | 1322 | CD2 | LEU | 182 | 137.414 | 13.405 | 59.808 | 1.00 | 5.44 |
| | 1323 | C | LEU | 182 | 140.164 | 16.760 | 60.884 | 1.00 | 23.01 |
| | 1324 | O | LEU | 182 | 140.177 | 17.787 | 61.567 | 1.00 | 24.75 |
| | 1325 | N | LYS | 183 | 141.071 | 16.492 | 59.953 | 1.00 | 23.75 |
| | 1326 | CA | LYS | 183 | 142.139 | 17.426 | 59.646 | 1.00 | 25.95 |
| 35 | 1327 | CB | LYS | 183 | 143.300 | 16.712 | 58.948 | 1.00 | 25.08 |
| | 1328 | CG | LYS | 183 | 142.946 | 16.106 | 57.600 | 1.00 | 32.88 |
| | 1329 | CD | LYS | 183 | 144.157 | 15.465 | 56.949 | 1.00 | 39.75 |
| | 1330 | CE | LYS | 183 | 143.804 | 14.905 | 55.581 | 1.00 | 45.64 |
| | 1331 | NZ | LYS | 183 | 144.980 | 14.277 | 54.913 | 1.00 | 50.66 |
| 40 | 1332 | C | LYS | 183 | 141.590 | 18.522 | 58.747 | 1.00 | 26.52 |
| | 1333 | O | LYS | 183 | 140.579 | 18.333 | 58.068 | 1.00 | 31.05 |
| | 1334 | N | SER | 184 | 142.247 | 19.675 | 58.769 | 1.00 | 25.24 |
| | 1335 | CA | SER | 184 | 141.842 | 20.806 | 57.949 | 1.00 | 18.75 |
| | 1336 | CB | SER | 184 | 142.202 | 22.111 | 58.656 | 1.00 | 15.62 |
| | 1337 | OG | SER | 184 | 141.536 | 22.192 | 59.906 | 1.00 | 17.72 |
| 45 | 1338 | C | SER | 184 | 142.553 | 20.707 | 56.605 | 1.00 | 13.85 |
| | 1339 | O | SER | 184 | 143.666 | 20.186 | 56.528 | 1.00 | 23.56 |
| | 1340 | N | PRO | 185 | 141.930 | 21.221 | 55.526 | 1.00 | 14.69 |
| | 1341 | CD | PRO | 185 | 142.636 | 21.342 | 54.235 | 1.00 | 6.08 |
| | 1342 | CA | PRO | 185 | 140.622 | 21.886 | 55.462 | 1.00 | 13.32 |
| 50 | 1343 | CB | PRO | 185 | 140.758 | 22.747 | 54.213 | 1.00 | 7.14 |

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|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 1344 | CG | PRO | 185 | 141.553 | 21.860 | 53.309 | 1.00 | 4.25 |
| | 1345 | C | PRO | 185 | 139.378 | 20.990 | 55.368 | 1.00 | 19.26 |
| | 1346 | O | PRO | 185 | 138.268 | 21.502 | 55.198 | 1.00 | 22.11 |
| 5 | 1347 | N | LEU | 186 | 139.547 | 19.671 | 55.478 | 1.00 | 15.43 |
| | 1348 | CA | LEU | 186 | 138.410 | 18.757 | 55.385 | 1.00 | 7.82 |
| | 1349 | CB | LEU | 186 | 138.859 | 17.304 | 55.533 | 1.00 | 10.45 |
| | 1350 | CG | LEU | 186 | 137.743 | 16.259 | 55.379 | 1.00 | 14.68 |
| | 1351 | CD1 | LEU | 186 | 137.199 | 16.257 | 53.953 | 1.00 | 2.00 |
| | 1352 | CD2 | LEU | 186 | 138.269 | 14.885 | 55.744 | 1.00 | 10.39 |
| 10 | 1353 | C | LEU | 186 | 137.339 | 19.061 | 56.424 | 1.00 | 14.43 |
| | 1354 | O | LEU | 186 | 136.147 | 19.062 | 56.114 | 1.00 | 15.11 |
| | 1355 | N | ARG | 187 | 137.774 | 19.318 | 57.653 | 1.00 | 11.19 |
| | 1356 | CA | ARG | 187 | 136.868 | 19.626 | 58.755 | 1.00 | 10.77 |
| | 1357 | CB | ARG | 187 | 137.675 | 19.929 | 60.019 | 1.00 | 9.64 |
| 15 | 1358 | CG | ARG | 187 | 136.839 | 20.202 | 61.251 | 1.00 | 12.29 |
| | 1359 | CD | ARG | 187 | 137.724 | 20.530 | 62.429 | 1.00 | 17.99 |
| | 1360 | NE | ARG | 187 | 136.944 | 20.796 | 63.633 | 1.00 | 40.99 |
| | 1361 | CZ | ARG | 187 | 137.468 | 20.982 | 64.841 | 1.00 | 53.63 |
| | 1362 | NH1 | ARG | 187 | 138.785 | 20.931 | 65.014 | 1.00 | 54.42 |
| 20 | 1363 | NH2 | ARG | 187 | 136.674 | 21.217 | 65.879 | 1.00 | 49.07 |
| | 1364 | C | ARG | 187 | 135.949 | 20.804 | 58.424 | 1.00 | 19.68 |
| | 1365 | O | ARG | 187 | 134.754 | 20.771 | 58.731 | 1.00 | 20.19 |
| | 1366 | N | GLU | 188 | 136.512 | 21.831 | 57.789 | 1.00 | 19.04 |
| | 1367 | CA | GLU | 188 | 135.758 | 23.026 | 57.405 | 1.00 | 14.75 |
| 25 | 1368 | CB | GLU | 188 | 136.708 | 24.179 | 57.052 | 1.00 | 18.38 |
| | 1369 | CG | GLU | 188 | 137.416 | 24.825 | 58.248 | 1.00 | 25.44 |
| | 1370 | CD | GLU | 188 | 138.326 | 23.865 | 59.000 | 1.00 | 37.02 |
| | 1371 | OE1 | GLU | 188 | 138.143 | 23.708 | 60.228 | 1.00 | 36.96 |
| | 1372 | OE2 | GLU | 188 | 139.224 | 23.271 | 58.362 | 1.00 | 33.70 |
| 30 | 1373 | C | GLU | 188 | 134.819 | 22.758 | 56.236 | 1.00 | 15.06 |
| | 1374 | O | GLU | 188 | 133.720 | 23.317 | 56.176 | 1.00 | 16.38 |
| | 1375 | N | GLN | 189 | 135.263 | 21.920 | 55.301 | 1.00 | 12.50 |
| | 1376 | CA | GLN | 189 | 134.458 | 21.567 | 54.134 | 1.00 | 10.80 |
| | 1377 | CB | GLN | 189 | 135.269 | 20.711 | 53.153 | 1.00 | 10.38 |
| 35 | 1378 | CG | GLN | 189 | 134.529 | 20.384 | 51.856 | 1.00 | 9.35 |
| | 1379 | CD | GLN | 189 | 135.415 | 19.722 | 50.811 | 1.00 | 16.04 |
| | 1380 | OE1 | GLN | 189 | 135.319 | 20.022 | 49.617 | 1.00 | 8.08 |
| | 1381 | NE2 | GLN | 189 | 136.277 | 18.812 | 51.254 | 1.00 | 11.78 |
| | 1382 | C | GLN | 189 | 133.204 | 20.814 | 54.574 | 1.00 | 12.51 |
| 40 | 1383 | O | GLN | 189 | 132.117 | 21.057 | 54.059 | 1.00 | 19.40 |
| | 1384 | N | VAL | 190 | 133.363 | 19.920 | 55.546 | 1.00 | 11.87 |
| | 1385 | CA | VAL | 190 | 132.250 | 19.139 | 56.070 | 1.00 | 14.05 |
| | 1386 | CB | VAL | 190 | 132.750 | 17.975 | 56.967 | 1.00 | 18.34 |
| | 1387 | CG1 | VAL | 190 | 131.574 | 17.265 | 57.637 | 1.00 | 19.94 |
| 45 | 1388 | CG2 | VAL | 190 | 133.556 | 16.986 | 56.135 | 1.00 | 2.59 |
| | 1389 | C | VAL | 190 | 131.300 | 20.031 | 56.865 | 1.00 | 12.69 |
| | 1390 | O | VAL | 190 | 130.091 | 20.012 | 56.642 | 1.00 | 16.38 |
| | 1391 | N | THR | 191 | 131.858 | 20.822 | 57.777 | 1.00 | 19.11 |
| | 1392 | CA | THR | 191 | 131.065 | 21.727 | 58.606 | 1.00 | 20.76 |
| 50 | 1393 | CB | THR | 191 | 131.964 | 22.557 | 59.551 | 1.00 | 23.59 |

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|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 1394 | OG1 | THR | 191 | 132.681 | 21.675 | 60.424 | 1.00 | 29.20 |
| | 1395 | CG2 | THR | 191 | 131.130 | 23.511 | 60.391 | 1.00 | 29.68 |
| | 1396 | C | THR | 191 | 130.241 | 22.664 | 57.731 | 1.00 | 19.82 |
| 5 | 1397 | O | THR | 191 | 129.073 | 22.927 | 58.023 | 1.00 | 24.05 |
| | 1398 | N | HIS | 192 | 130.843 | 23.136 | 56.641 | 1.00 | 11.94 |
| | 1399 | CA | HIS | 192 | 130.160 | 24.032 | 55.719 | 1.00 | 13.13 |
| | 1400 | CB | HIS | 192 | 131.148 | 24.658 | 54.741 | 1.00 | 14.49 |
| | 1401 | CG | HIS | 192 | 130.512 | 25.600 | 53.764 | 1.00 | 13.85 |
| 10 | 1402 | CD2 | HIS | 192 | 130.320 | 25.503 | 52.428 | 1.00 | 14.30 |
| | 1403 | ND1 | HIS | 192 | 129.981 | 26.814 | 54.141 | 1.00 | 17.04 |
| | 1404 | CE1 | HIS | 192 | 129.488 | 27.425 | 53.078 | 1.00 | 22.40 |
| | 1405 | NE2 | HIS | 192 | 129.681 | 26.651 | 52.025 | 1.00 | 9.94 |
| | 1406 | C | HIS | 192 | 129.061 | 23.321 | 54.939 | 1.00 | 15.72 |
| 15 | 1407 | O | HIS | 192 | 128.002 | 23.896 | 54.696 | 1.00 | 19.37 |
| | 1408 | N | ALA | 193 | 129.331 | 22.085 | 54.524 | 1.00 | 22.40 |
| | 1409 | CA | ALA | 193 | 128.367 | 21.288 | 53.766 | 1.00 | 17.47 |
| | 1410 | CB | ALA | 193 | 128.993 | 19.976 | 53.333 | 1.00 | 13.16 |
| | 1411 | C | ALA | 193 | 127.104 | 21.027 | 54.584 | 1.00 | 18.46 |
| 20 | 1412 | O | ALA | 193 | 125.991 | 21.093 | 54.063 | 1.00 | 20.11 |
| | 1413 | N | LEU | 194 | 127.285 | 20.747 | 55.870 | 1.00 | 13.26 |
| | 1414 | CA | LEU | 194 | 126.165 | 20.488 | 56.763 | 1.00 | 18.67 |
| | 1415 | CB | LEU | 194 | 126.669 | 19.948 | 58.103 | 1.00 | 22.98 |
| | 1416 | CG | LEU | 194 | 127.424 | 18.615 | 58.050 | 1.00 | 17.83 |
| 25 | 1417 | CD1 | LEU | 194 | 127.913 | 18.249 | 59.439 | 1.00 | 22.28 |
| | 1418 | CD2 | LEU | 194 | 126.526 | 17.524 | 57.494 | 1.00 | 9.41 |
| | 1419 | C | LEU | 194 | 125.325 | 21.745 | 56.977 | 1.00 | 20.18 |
| | 1420 | O | LEU | 194 | 124.169 | 21.662 | 57.390 | 1.00 | 28.31 |
| | 1421 | N | GLU | 195 | 125.913 | 22.906 | 56.701 | 1.00 | 23.69 |
| 30 | 1422 | CA | GLU | 195 | 125.217 | 24.182 | 56.845 | 1.00 | 23.91 |
| | 1423 | CB | GLU | 195 | 126.145 | 25.235 | 57.459 | 1.00 | 28.38 |
| | 1424 | CG | GLU | 195 | 126.558 | 24.930 | 58.897 | 1.00 | 48.57 |
| | 1425 | CD | GLU | 195 | 127.591 | 25.905 | 59.449 | 1.00 | 61.92 |
| | 1426 | OE1 | GLU | 195 | 128.341 | 26.515 | 58.652 | 1.00 | 66.87 |
| 35 | 1427 | OE2 | GLU | 195 | 127.658 | 26.052 | 60.690 | 1.00 | 55.96 |
| | 1428 | C | GLU | 195 | 124.693 | 24.670 | 55.497 | 1.00 | 14.54 |
| | 1429 | O | GLU | 195 | 123.721 | 25.422 | 55.436 | 1.00 | 17.77 |
| | 1430 | N | GLN | 196 | 125.327 | 24.207 | 54.422 | 1.00 | 10.51 |
| | 1431 | CA | GLN | 196 | 124.951 | 24.584 | 53.064 | 1.00 | 9.57 |
| 40 | 1432 | CB | GLN | 196 | 125.488 | 25.984 | 52.740 | 1.00 | 9.74 |
| | 1433 | CG | GLN | 196 | 125.212 | 26.461 | 51.321 | 1.00 | 13.51 |
| | 1434 | CD | GLN | 196 | 123.737 | 26.672 | 51.051 | 1.00 | 18.27 |
| | 1435 | OE1 | GLN | 196 | 123.111 | 27.556 | 51.633 | 1.00 | 31.94 |
| | 1436 | NE2 | GLN | 196 | 123.174 | 25.862 | 50.162 | 1.00 | 21.35 |
| 45 | 1437 | C | GLN | 196 | 125.484 | 23.583 | 52.039 | 1.00 | 8.87 |
| | 1438 | O | GLN | 196 | 126.695 | 23.481 | 51.830 | 1.00 | 16.57 |
| | 1439 | N | CYS | 197 | 124.577 | 22.837 | 51.415 | 1.00 | 11.72 |
| | 1440 | CA | CYS | 197 | 124.963 | 21.865 | 50.398 | 1.00 | 13.36 |
| | 1441 | CB | CYS | 197 | 123.821 | 20.882 | 50.114 | 1.00 | 20.25 |
| 50 | 1442 | SG | CYS | 197 | 122.310 | 21.605 | 49.432 | 1.00 | 16.36 |
| | 1443 | C | CYS | 197 | 125.351 | 22.614 | 49.126 | 1.00 | 11.32 |

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|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 1444 | O | CYS | 197 | 124.948 | 23.758 | 48.924 | 1.00 | 16.69 |
| | 1445 | N | LEU | 198 | 126.134 | 21.965 | 48.274 | 1.00 | 14.40 |
| | 1446 | CA | LEU | 198 | 126.594 | 22.580 | 47.038 | 1.00 | 14.31 |
| | 1447 | CB | LEU | 198 | 127.688 | 21.717 | 46.394 | 1.00 | 14.46 |
| 5 | 1448 | CG | LEU | 198 | 128.283 | 22.186 | 45.060 | 1.00 | 13.58 |
| | 1449 | CD1 | LEU | 198 | 128.949 | 23.541 | 45.225 | 1.00 | 9.55 |
| | 1450 | CD2 | LEU | 198 | 129.279 | 21.162 | 44.547 | 1.00 | 12.33 |
| | 1451 | C | LEU | 198 | 125.478 | 22.848 | 46.034 | 1.00 | 18.46 |
| | 1452 | O | LEU | 198 | 125.389 | 23.945 | 45.481 | 1.00 | 26.64 |
| 10 | 1453 | N | HIS | 199 | 124.614 | 21.857 | 45.829 | 1.00 | 20.84 |
| | 1454 | CA | HIS | 199 | 123.519 | 21.965 | 44.869 | 1.00 | 13.67 |
| | 1455 | CB | HIS | 199 | 122.756 | 20.640 | 44.781 | 1.00 | 11.33 |
| | 1456 | CG | HIS | 199 | 121.733 | 20.603 | 43.688 | 1.00 | 6.17 |
| | 1457 | CD2 | HIS | 199 | 120.389 | 20.445 | 43.729 | 1.00 | 12.38 |
| 15 | 1458 | ND1 | HIS | 199 | 122.061 | 20.738 | 42.356 | 1.00 | 10.08 |
| | 1459 | CE1 | HIS | 199 | 120.964 | 20.663 | 41.624 | 1.00 | 10.18 |
| | 1460 | NE2 | HIS | 199 | 119.935 | 20.486 | 42.432 | 1.00 | 2.01 |
| | 1461 | C | HIS | 199 | 122.540 | 23.111 | 45.108 | 1.00 | 14.52 |
| | 1462 | O | HIS | 199 | 122.174 | 23.813 | 44.166 | 1.00 | 13.39 |
| 20 | 1463 | N | LYS | 200 | 122.120 | 23.300 | 46.357 | 1.00 | 15.92 |
| | 1464 | CA | LYS | 200 | 121.161 | 24.353 | 46.698 | 1.00 | 14.65 |
| | 1465 | CB | LYS | 200 | 120.205 | 23.859 | 47.789 | 1.00 | 15.18 |
| | 1466 | CG | LYS | 200 | 119.425 | 22.609 | 47.416 | 1.00 | 12.45 |
| | 1467 | CD | LYS | 200 | 118.523 | 22.158 | 48.554 | 1.00 | 3.23 |
| 25 | 1468 | CE | LYS | 200 | 117.827 | 20.849 | 48.213 | 1.00 | 14.66 |
| | 1469 | NZ | LYS | 200 | 116.966 | 20.369 | 49.332 | 1.00 | 22.03 |
| | 1470 | C | LYS | 200 | 121.786 | 25.688 | 47.120 | 1.00 | 22.11 |
| | 1471 | O | LYS | 200 | 121.101 | 26.541 | 47.693 | 1.00 | 20.41 |
| | 1472 | N | GLY | 201 | 123.078 | 25.860 | 46.844 | 1.00 | 21.90 |
| 30 | 1473 | CA | GLY | 201 | 123.764 | 27.097 | 47.191 | 1.00 | 14.85 |
| | 1474 | C | GLY | 201 | 124.048 | 27.969 | 45.978 | 1.00 | 16.72 |
| | 1475 | O | GLY | 201 | 123.992 | 27.489 | 44.842 | 1.00 | 12.09 |
| | 1476 | N | VAL | 202 | 124.329 | 29.253 | 46.209 | 1.00 | 11.53 |
| | 1477 | CA | VAL | 202 | 124.627 | 30.183 | 45.114 | 1.00 | 11.31 |
| 35 | 1478 | CB | VAL | 202 | 124.437 | 31.661 | 45.555 | 1.00 | 9.93 |
| | 1479 | CG1 | VAL | 202 | 124.960 | 32.617 | 44.491 | 1.00 | 2.00 |
| | 1480 | CG2 | VAL | 202 | 122.964 | 31.937 | 45.803 | 1.00 | 6.34 |
| | 1481 | C | VAL | 202 | 126.054 | 29.940 | 44.612 | 1.00 | 10.17 |
| | 1482 | O | VAL | 202 | 126.997 | 29.883 | 45.405 | 1.00 | 8.95 |
| 40 | 1483 | N | PRO | 203 | 126.222 | 29.774 | 43.286 | 1.00 | 2.10 |
| | 1484 | CD | PRO | 203 | 125.136 | 29.796 | 42.290 | 1.00 | 5.19 |
| | 1485 | CA | PRO | 203 | 127.509 | 29.524 | 42.628 | 1.00 | 8.34 |
| | 1486 | CB | PRO | 203 | 127.168 | 29.704 | 41.154 | 1.00 | 5.82 |
| | 1487 | CG | PRO | 203 | 125.785 | 29.152 | 41.087 | 1.00 | 2.00 |
| 45 | 1488 | C | PRO | 203 | 128.699 | 30.381 | 43.069 | 1.00 | 18.54 |
| | 1489 | O | PRO | 203 | 129.709 | 29.836 | 43.516 | 1.00 | 26.42 |
| | 1490 | N | ARG | 204 | 128.591 | 31.704 | 42.951 | 1.00 | 11.17 |
| | 1491 | CA | ARG | 204 | 129.687 | 32.582 | 43.357 | 1.00 | 5.94 |
| | 1492 | CB | ARG | 204 | 129.366 | 34.047 | 43.061 | 1.00 | 4.29 |
| 50 | 1493 | CG | ARG | 204 | 129.405 | 34.440 | 41.587 | 1.00 | 10.69 |

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|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 1494 | CD | ARG | 204 | 130.821 | 34.543 | 41.033 | 1.00 | 8.35 |
| | 1495 | NE | ARG | 204 | 131.410 | 33.242 | 40.725 | 1.00 | 21.05 |
| | 1496 | CZ | ARG | 204 | 132.555 | 33.071 | 40.068 | 1.00 | 20.78 |
| 5 | 1497 | NH1 | ARG | 204 | 133.250 | 34.121 | 39.644 | 1.00 | 14.75 |
| | 1498 | NH2 | ARG | 204 | 132.996 | 31.844 | 39.818 | 1.00 | 16.69 |
| | 1499 | C | ARG | 204 | 130.016 | 32.420 | 44.836 | 1.00 | 6.43 |
| | 1500 | O | ARG | 204 | 131.185 | 32.304 | 45.207 | 1.00 | 15.01 |
| | 1501 | N | VAL | 205 | 128.983 | 32.380 | 45.672 | 1.00 | 2.00 |
| 10 | 1502 | CA | VAL | 205 | 129.159 | 32.238 | 47.116 | 1.00 | 3.42 |
| | 1503 | CB | VAL | 205 | 127.809 | 32.238 | 47.855 | 1.00 | 2.00 |
| | 1504 | CG1 | VAL | 205 | 128.027 | 32.047 | 49.342 | 1.00 | 13.49 |
| | 1505 | CG2 | VAL | 205 | 127.064 | 33.530 | 47.594 | 1.00 | 2.00 |
| | 1506 | C | VAL | 205 | 129.904 | 30.963 | 47.488 | 1.00 | 7.19 |
| 15 | 1507 | O | VAL | 205 | 130.785 | 30.982 | 48.342 | 1.00 | 17.39 |
| | 1508 | N | GLU | 206 | 129.543 | 29.854 | 46.851 | 1.00 | 11.33 |
| | 1509 | CA | GLU | 206 | 130.188 | 28.579 | 47.136 | 1.00 | 11.44 |
| | 1510 | CB | GLU | 206 | 129.348 | 27.417 | 46.606 | 1.00 | 10.75 |
| | 1511 | CG | GLU | 206 | 128.033 | 27.237 | 47.340 | 1.00 | 4.42 |
| 20 | 1512 | CD | GLU | 206 | 128.208 | 27.226 | 48.845 | 1.00 | 7.68 |
| | 1513 | OE1 | GLU | 206 | 128.858 | 26.298 | 49.366 | 1.00 | 15.79 |
| | 1514 | OE2 | GLU | 206 | 127.700 | 28.153 | 49.509 | 1.00 | 12.42 |
| | 1515 | C | GLU | 206 | 131.598 | 28.528 | 46.568 | 1.00 | 13.88 |
| | 1516 | O | GLU | 206 | 132.484 | 27.897 | 47.144 | 1.00 | 16.22 |
| 25 | 1517 | N | THR | 207 | 131.792 | 29.199 | 45.438 | 1.00 | 9.73 |
| | 1518 | CA | THR | 207 | 133.090 | 29.268 | 44.785 | 1.00 | 13.84 |
| | 1519 | CB | THR | 207 | 132.970 | 29.928 | 43.400 | 1.00 | 15.72 |
| | 1520 | OG1 | THR | 207 | 132.272 | 29.045 | 42.513 | 1.00 | 13.12 |
| | 1521 | CG2 | THR | 207 | 134.338 | 30.250 | 42.827 | 1.00 | 11.92 |
| 30 | 1522 | C | THR | 207 | 134.059 | 30.066 | 45.658 | 1.00 | 19.41 |
| | 1523 | O | THR | 207 | 135.177 | 29.623 | 45.917 | 1.00 | 27.17 |
| | 1524 | N | ARG | 208 | 133.608 | 31.226 | 46.133 | 1.00 | 22.15 |
| | 1525 | CA | ARG | 208 | 134.417 | 32.091 | 46.988 | 1.00 | 17.49 |
| | 1526 | CB | ARG | 208 | 133.595 | 33.309 | 47.429 | 1.00 | 23.71 |
| 35 | 1527 | CG | ARG | 208 | 134.349 | 34.352 | 48.264 | 1.00 | 24.20 |
| | 1528 | CD | ARG | 208 | 135.532 | 34.935 | 47.501 | 1.00 | 35.41 |
| | 1529 | NE | ARG | 208 | 136.060 | 36.169 | 48.090 | 1.00 | 40.81 |
| | 1530 | CZ | ARG | 208 | 136.736 | 36.242 | 49.235 | 1.00 | 40.71 |
| | 1531 | NH1 | ARG | 208 | 136.978 | 35.150 | 49.947 | 1.00 | 42.82 |
| 40 | 1532 | NH2 | ARG | 208 | 137.194 | 37.412 | 49.658 | 1.00 | 37.98 |
| | 1533 | C | ARG | 208 | 134.906 | 31.313 | 48.208 | 1.00 | 19.76 |
| | 1534 | O | ARG | 208 | 136.075 | 31.395 | 48.576 | 1.00 | 27.03 |
| | 1535 | N | PHE | 209 | 134.010 | 30.534 | 48.809 | 1.00 | 16.90 |
| | 1536 | CA | PHE | 209 | 134.350 | 29.734 | 49.979 | 1.00 | 12.93 |
| 45 | 1537 | CB | PHE | 209 | 133.090 | 29.165 | 50.632 | 1.00 | 3.91 |
| | 1538 | CG | PHE | 209 | 133.377 | 28.292 | 51.818 | 1.00 | 8.27 |
| | 1539 | CD1 | PHE | 209 | 133.605 | 28.852 | 53.070 | 1.00 | 5.35 |
| | 1540 | CD2 | PHE | 209 | 133.472 | 26.912 | 51.676 | 1.00 | 11.24 |
| | 1541 | CE1 | PHE | 209 | 133.928 | 28.052 | 54.162 | 1.00 | 10.99 |
| | 1542 | CE2 | PHE | 209 | 133.794 | 26.105 | 52.760 | 1.00 | 7.23 |
| 50 | 1543 | CZ | PHE | 209 | 134.023 | 26.677 | 54.007 | 1.00 | 2.00 |

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|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 1544 | C | PHE | 209 | 135.305 | 28.581 | 49.664 | 1.00 | 16.94 |
| | 1545 | O | PHE | 209 | 136.176 | 28.248 | 50.473 | 1.00 | 13.43 |
| | 1546 | N | PHE | 210 | 135.112 | 27.942 | 48.514 | 1.00 | 11.91 |
| | 1547 | CA | PHE | 210 | 135.960 | 26.823 | 48.126 | 1.00 | 12.01 |
| 5 | 1548 | CB | PHE | 210 | 135.384 | 26.105 | 46.901 | 1.00 | 5.35 |
| | 1549 | CG | PHE | 210 | 136.131 | 24.854 | 46.525 | 1.00 | 2.00 |
| | 1550 | CD1 | PHE | 210 | 136.182 | 23.773 | 47.392 | 1.00 | 7.13 |
| | 1551 | CD2 | PHE | 210 | 136.794 | 24.763 | 45.307 | 1.00 | 13.50 |
| | 1552 | CE1 | PHE | 210 | 136.883 | 22.617 | 47.052 | 1.00 | 13.12 |
| 10 | 1553 | CE2 | PHE | 210 | 137.498 | 23.613 | 44.956 | 1.00 | 10.64 |
| | 1554 | CZ | PHE | 210 | 137.542 | 22.539 | 45.830 | 1.00 | 12.55 |
| | 1555 | C | PHE | 210 | 137.380 | 27.297 | 47.844 | 1.00 | 15.50 |
| | 1556 | O | PHE | 210 | 138.339 | 26.801 | 48.436 | 1.00 | 21.01 |
| | 1557 | N | ILE | 211 | 137.500 | 28.290 | 46.970 | 1.00 | 11.89 |
| 15 | 1558 | CA | ILE | 211 | 138.798 | 28.834 | 46.601 | 1.00 | 14.18 |
| | 1559 | CB | ILE | 211 | 138.663 | 30.000 | 45.604 | 1.00 | 13.95 |
| | 1560 | CG2 | ILE | 211 | 140.040 | 30.517 | 45.218 | 1.00 | 23.94 |
| | 1561 | CG1 | ILE | 211 | 137.925 | 29.547 | 44.346 | 1.00 | 14.06 |
| | 1562 | CD1 | ILE | 211 | 137.734 | 30.656 | 43.335 | 1.00 | 19.84 |
| 20 | 1563 | C | ILE | 211 | 139.622 | 29.318 | 47.790 | 1.00 | 11.48 |
| | 1564 | O | ILE | 211 | 140.730 | 28.838 | 48.010 | 1.00 | 22.99 |
| | 1565 | N | SER | 212 | 139.069 | 30.238 | 48.574 | 1.00 | 11.99 |
| | 1566 | CA | SER | 212 | 139.799 | 30.797 | 49.708 | 1.00 | 19.48 |
| | 1567 | CB | SER | 212 | 139.279 | 32.205 | 50.044 | 1.00 | 10.83 |
| 25 | 1568 | OG | SER | 212 | 137.939 | 32.174 | 50.500 | 1.00 | 32.56 |
| | 1569 | C | SER | 212 | 139.902 | 29.954 | 50.979 | 1.00 | 15.60 |
| | 1570 | O | SER | 212 | 140.992 | 29.800 | 51.530 | 1.00 | 26.35 |
| | 1571 | N | SER | 213 | 138.785 | 29.398 | 51.437 | 1.00 | 18.79 |
| | 1572 | CA | SER | 213 | 138.780 | 28.607 | 52.665 | 1.00 | 15.21 |
| 30 | 1573 | CB | SER | 213 | 137.426 | 28.737 | 53.372 | 1.00 | 13.39 |
| | 1574 | OG | SER | 213 | 137.168 | 30.074 | 53.766 | 1.00 | 19.66 |
| | 1575 | C | SER | 213 | 139.141 | 27.126 | 52.543 | 1.00 | 21.19 |
| | 1576 | O | SER | 213 | 139.540 | 26.503 | 53.534 | 1.00 | 22.69 |
| | 1577 | N | ILE | 214 | 139.021 | 26.558 | 51.345 | 1.00 | 16.22 |
| 35 | 1578 | CA | ILE | 214 | 139.308 | 25.138 | 51.177 | 1.00 | 12.65 |
| | 1579 | CB | ILE | 214 | 138.047 | 24.354 | 50.712 | 1.00 | 17.01 |
| | 1580 | CG2 | ILE | 214 | 138.343 | 22.853 | 50.628 | 1.00 | 14.54 |
| | 1581 | CG1 | ILE | 214 | 136.879 | 24.602 | 51.673 | 1.00 | 7.09 |
| | 1582 | CD1 | ILE | 214 | 137.175 | 24.247 | 53.124 | 1.00 | 2.16 |
| 40 | 1583 | C | ILE | 214 | 140.477 | 24.759 | 50.276 | 1.00 | 14.51 |
| | 1584 | O | ILE | 214 | 141.486 | 24.247 | 50.759 | 1.00 | 20.94 |
| | 1585 | N | TYR | 215 | 140.342 | 25.006 | 48.975 | 1.00 | 10.71 |
| | 1586 | CA | TYR | 215 | 141.378 | 24.634 | 48.016 | 1.00 | 16.76 |
| | 1587 | CB | TYR | 215 | 140.914 | 24.914 | 46.587 | 1.00 | 10.15 |
| 45 | 1588 | CG | TYR | 215 | 141.523 | 23.975 | 45.569 | 1.00 | 16.49 |
| | 1589 | CD1 | TYR | 215 | 141.526 | 22.595 | 45.777 | 1.00 | 14.36 |
| | 1590 | CE1 | TYR | 215 | 142.079 | 21.722 | 44.837 | 1.00 | 16.84 |
| | 1591 | CD2 | TYR | 215 | 142.090 | 24.463 | 44.393 | 1.00 | 18.93 |
| | 1592 | CE2 | TYR | 215 | 142.645 | 23.601 | 43.447 | 1.00 | 14.61 |
| 50 | 1593 | CZ | TYR | 215 | 142.636 | 22.232 | 43.676 | 1.00 | 18.72 |

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|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 1594 | OH | TYR | 215 | 143.191 | 21.375 | 42.749 | 1.00 | 21.97 |
| | 1595 | C | TYR | 215 | 142.753 | 25.251 | 48.256 | 1.00 | 22.56 |
| | 1596 | O | TYR | 215 | 143.772 | 24.567 | 48.154 | 1.00 | 21.88 |
| | 1597 | N | ASP | 216 | 142.780 | 26.538 | 48.582 | 1.00 | 25.86 |
| 5 | 1598 | CA | ASP | 216 | 144.032 | 27.239 | 48.841 | 1.00 | 28.90 |
| | 1599 | CB | ASP | 216 | 143.745 | 28.708 | 49.155 | 1.00 | 35.55 |
| | 1600 | CG | ASP | 216 | 145.000 | 29.514 | 49.373 | 1.00 | 32.91 |
| | 1601 | OD1 | ASP | 216 | 145.170 | 30.035 | 50.494 | 1.00 | 33.80 |
| | 1602 | OD2 | ASP | 216 | 145.811 | 29.630 | 48.427 | 1.00 | 38.29 |
| 10 | 1603 | C | ASP | 216 | 144.782 | 26.590 | 50.002 | 1.00 | 28.68 |
| | 1604 | O | ASP | 216 | 146.013 | 26.552 | 50.017 | 1.00 | 35.11 |
| | 1605 | N | LYS | 217 | 144.026 | 26.052 | 50.954 | 1.00 | 24.04 |
| | 1606 | CA | LYS | 217 | 144.604 | 25.406 | 52.129 | 1.00 | 25.31 |
| | 1607 | CB | LYS | 217 | 143.768 | 25.741 | 53.368 | 1.00 | 17.45 |
| 15 | 1608 | CG | LYS | 217 | 143.687 | 27.234 | 53.646 | 1.00 | 28.42 |
| | 1609 | CD | LYS | 217 | 142.811 | 27.551 | 54.844 | 1.00 | 36.77 |
| | 1610 | CE | LYS | 217 | 142.729 | 29.057 | 55.071 | 1.00 | 36.92 |
| | 1611 | NZ | LYS | 217 | 141.758 | 29.426 | 56.143 | 1.00 | 37.10 |
| | 1612 | C | LYS | 217 | 144.754 | 23.892 | 51.973 | 1.00 | 25.97 |
| 20 | 1613 | O | LYS | 217 | 145.170 | 23.201 | 52.905 | 1.00 | 23.71 |
| | 1614 | N | GLU | 218 | 144.429 | 23.385 | 50.788 | 1.00 | 30.40 |
| | 1615 | CA | GLU | 218 | 144.528 | 21.958 | 50.504 | 1.00 | 34.37 |
| | 1616 | CB | GLU | 218 | 143.655 | 21.603 | 49.297 | 1.00 | 41.93 |
| | 1617 | CG | GLU | 218 | 143.462 | 20.114 | 49.073 | 1.00 | 45.33 |
| 25 | 1618 | CD | GLU | 218 | 142.740 | 19.451 | 50.226 | 1.00 | 52.39 |
| | 1619 | OE1 | GLU | 218 | 141.553 | 19.780 | 50.449 | 1.00 | 49.41 |
| | 1620 | OE2 | GLU | 218 | 143.364 | 18.612 | 50.916 | 1.00 | 46.07 |
| | 1621 | C | GLU | 218 | 145.982 | 21.585 | 50.228 | 1.00 | 34.68 |
| | 1622 | O | GLU | 218 | 146.624 | 22.166 | 49.356 | 1.00 | 31.92 |
| 30 | 1623 | N | GLN | 219 | 146.493 | 20.611 | 50.974 | 1.00 | 37.87 |
| | 1624 | CA | GLN | 219 | 147.872 | 20.156 | 50.827 | 1.00 | 41.61 |
| | 1625 | CB | GLN | 219 | 148.180 | 19.105 | 51.896 | 1.00 | 52.08 |
| | 1626 | CG | GLN | 219 | 149.617 | 18.615 | 51.900 | 1.00 | 67.09 |
| | 1627 | CD | GLN | 219 | 149.709 | 17.102 | 51.943 | 1.00 | 78.27 |
| 35 | 1628 | OE1 | GLN | 219 | 149.305 | 16.470 | 52.917 | 1.00 | 81.71 |
| | 1629 | NE2 | GLN | 219 | 150.233 | 16.510 | 50.870 | 1.00 | 80.10 |
| | 1630 | C | GLN | 219 | 148.173 | 19.583 | 49.438 | 1.00 | 38.79 |
| | 1631 | O | GLN | 219 | 149.260 | 19.789 | 48.893 | 1.00 | 34.89 |
| | 1632 | N | SER | 220 | 147.205 | 18.867 | 48.874 | 1.00 | 39.35 |
| 40 | 1633 | CA | SER | 220 | 147.359 | 18.252 | 47.556 | 1.00 | 36.65 |
| | 1634 | CB | SER | 220 | 146.658 | 16.891 | 47.537 | 1.00 | 48.69 |
| | 1635 | OG | SER | 220 | 145.291 | 17.018 | 47.899 | 1.00 | 58.57 |
| | 1636 | C | SER | 220 | 146.824 | 19.117 | 46.418 | 1.00 | 30.45 |
| | 1637 | O | SER | 220 | 146.651 | 18.639 | 45.297 | 1.00 | 31.98 |
| 45 | 1638 | N | LYS | 221 | 146.581 | 20.392 | 46.704 | 1.00 | 25.39 |
| | 1639 | CA | LYS | 221 | 146.052 | 21.327 | 45.716 | 1.00 | 18.20 |
| | 1640 | CB | LYS | 221 | 145.949 | 22.731 | 46.316 | 1.00 | 17.94 |
| | 1641 | CG | LYS | 221 | 147.292 | 23.352 | 46.659 | 1.00 | 24.63 |
| | 1642 | CD | LYS | 221 | 147.136 | 24.772 | 47.155 | 1.00 | 32.69 |
| 50 | 1643 | CE | LYS | 221 | 148.444 | 25.312 | 47.716 | 1.00 | 42.07 |

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|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 1644 | NZ | LYS | 221 | 149.547 | 25.257 | 46.720 | 1.00 | 42.25 |
| | 1645 | C | LYS | 221 | 146.879 | 21.412 | 44.444 | 1.00 | 15.22 |
| | 1646 | O | LYS | 221 | 148.097 | 21.243 | 44.467 | 1.00 | 21.32 |
| 5 | 1647 | N | ASN | 222 | 146.196 | 21.660 | 43.333 | 1.00 | 11.20 |
| | 1648 | CA | ASN | 222 | 146.853 | 21.818 | 42.048 | 1.00 | 9.54 |
| | 1649 | CB | ASN | 222 | 145.993 | 21.250 | 40.919 | 1.00 | 2.46 |
| | 1650 | CG | ASN | 222 | 146.599 | 21.488 | 39.550 | 1.00 | 12.07 |
| | 1651 | OD1 | ASN | 222 | 146.698 | 22.626 | 39.097 | 1.00 | 10.03 |
| 10 | 1652 | ND2 | ASN | 222 | 147.003 | 20.414 | 38.881 | 1.00 | 11.12 |
| | 1653 | C | ASN | 222 | 147.032 | 23.322 | 41.885 | 1.00 | 17.59 |
| | 1654 | O | ASN | 222 | 146.060 | 24.061 | 41.717 | 1.00 | 21.24 |
| | 1655 | N | ASN | 223 | 148.281 | 23.765 | 41.958 | 1.00 | 18.52 |
| | 1656 | CA | ASN | 223 | 148.619 | 25.175 | 41.850 | 1.00 | 9.91 |
| | 1657 | CB | ASN | 223 | 150.127 | 25.349 | 41.972 | 1.00 | 11.52 |
| 15 | 1658 | CG | ASN | 223 | 150.664 | 24.821 | 43.282 | 1.00 | 23.77 |
| | 1659 | OD1 | ASN | 223 | 150.579 | 25.491 | 44.311 | 1.00 | 21.40 |
| | 1660 | ND2 | ASN | 223 | 151.208 | 23.605 | 43.258 | 1.00 | 21.52 |
| | 1661 | C | ASN | 223 | 148.104 | 25.870 | 40.594 | 1.00 | 15.35 |
| | 1662 | O | ASN | 223 | 147.668 | 27.019 | 40.662 | 1.00 | 21.88 |
| 20 | 1663 | N | VAL | 224 | 148.157 | 25.184 | 39.455 | 1.00 | 10.58 |
| | 1664 | CA | VAL | 224 | 147.677 | 25.755 | 38.195 | 1.00 | 18.60 |
| | 1665 | CB | VAL | 224 | 147.957 | 24.811 | 37.001 | 1.00 | 24.63 |
| | 1666 | CG1 | VAL | 224 | 147.405 | 25.406 | 35.709 | 1.00 | 25.94 |
| | 1667 | CG2 | VAL | 224 | 149.449 | 24.558 | 36.873 | 1.00 | 17.27 |
| 25 | 1668 | C | VAL | 224 | 146.177 | 26.049 | 38.259 | 1.00 | 23.24 |
| | 1669 | O | VAL | 224 | 145.716 | 27.071 | 37.746 | 1.00 | 25.12 |
| | 1670 | N | LEU | 225 | 145.423 | 25.146 | 38.886 | 1.00 | 23.80 |
| | 1671 | CA | LEU | 225 | 143.980 | 25.313 | 39.032 | 1.00 | 18.51 |
| | 1672 | CB | LEU | 225 | 143.314 | 23.994 | 39.434 | 1.00 | 18.23 |
| 30 | 1673 | CG | LEU | 225 | 143.337 | 22.844 | 38.424 | 1.00 | 20.30 |
| | 1674 | CD1 | LEU | 225 | 142.613 | 21.645 | 39.010 | 1.00 | 18.77 |
| | 1675 | CD2 | LEU | 225 | 142.691 | 23.270 | 37.115 | 1.00 | 10.44 |
| | 1676 | C | LEU | 225 | 143.652 | 26.392 | 40.061 | 1.00 | 18.24 |
| | 1677 | O | LEU | 225 | 142.710 | 27.162 | 39.872 | 1.00 | 22.06 |
| 35 | 1678 | N | LEU | 226 | 144.431 | 26.448 | 41.141 | 1.00 | 18.51 |
| | 1679 | CA | LEU | 226 | 144.230 | 27.445 | 42.197 | 1.00 | 17.64 |
| | 1680 | CB | LEU | 226 | 145.128 | 27.149 | 43.401 | 1.00 | 15.88 |
| | 1681 | CG | LEU | 226 | 145.013 | 28.096 | 44.605 | 1.00 | 19.63 |
| | 1682 | CD1 | LEU | 226 | 143.633 | 27.996 | 45.235 | 1.00 | 8.24 |
| 40 | 1683 | CD2 | LEU | 226 | 146.086 | 27.764 | 45.627 | 1.00 | 2.89 |
| | 1684 | C | LEU | 226 | 144.507 | 28.855 | 41.681 | 1.00 | 15.54 |
| | 1685 | O | LEU | 226 | 143.753 | 29.785 | 41.966 | 1.00 | 28.19 |
| | 1686 | N | ARG | 227 | 145.595 | 29.002 | 40.927 | 1.00 | 22.25 |
| | 1687 | CA | ARG | 227 | 145.995 | 30.282 | 40.338 | 1.00 | 21.24 |
| 45 | 1688 | CB | ARG | 227 | 147.320 | 30.108 | 39.587 | 1.00 | 25.23 |
| | 1689 | CG | ARG | 227 | 147.831 | 31.335 | 38.844 | 1.00 | 26.56 |
| | 1690 | CD | ARG | 227 | 148.575 | 32.292 | 39.760 | 1.00 | 33.23 |
| | 1691 | NE | ARG | 227 | 149.114 | 33.433 | 39.021 | 1.00 | 27.48 |
| | 1692 | CZ | ARG | 227 | 149.516 | 34.568 | 39.585 | 1.00 | 29.44 |
| 50 | 1693 | NH1 | ARG | 227 | 149.447 | 34.722 | 40.902 | 1.00 | 31.95 |

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|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 1694 | NH2 | ARG | 227 | 149.963 | 35.561 | 38.831 | 1.00 | 19.58 |
| | 1695 | C | ARG | 227 | 144.911 | 30.745 | 39.367 | 1.00 | 17.48 |
| | 1696 | O | ARG | 227 | 144.475 | 31.894 | 39.402 | 1.00 | 22.08 |
| | 1697 | N | PHE | 228 | 144.474 | 29.822 | 38.516 | 1.00 | 17.49 |
| 5 | 1698 | CA | PHE | 228 | 143.439 | 30.073 | 37.516 | 1.00 | 20.78 |
| | 1699 | CB | PHE | 228 | 143.184 | 28.770 | 36.741 | 1.00 | 17.58 |
| | 1700 | CG | PHE | 228 | 142.261 | 28.908 | 35.556 | 1.00 | 10.74 |
| | 1701 | CD1 | PHE | 228 | 141.685 | 30.128 | 35.214 | 1.00 | 18.32 |
| | 1702 | CD2 | PHE | 228 | 141.958 | 27.791 | 34.785 | 1.00 | 13.57 |
| 10 | 1703 | CE1 | PHE | 228 | 140.819 | 30.230 | 34.122 | 1.00 | 18.76 |
| | 1704 | CE2 | PHE | 228 | 141.095 | 27.883 | 33.692 | 1.00 | 18.93 |
| | 1705 | CZ | PHE | 228 | 140.525 | 29.106 | 33.361 | 1.00 | 12.22 |
| | 1706 | C | PHE | 228 | 142.158 | 30.552 | 38.205 | 1.00 | 20.33 |
| | 1707 | O | PHE | 228 | 141.585 | 31.580 | 37.834 | 1.00 | 17.12 |
| 15 | 1708 | N | ALA | 229 | 141.746 | 29.817 | 39.233 | 1.00 | 15.85 |
| | 1709 | CA | ALA | 229 | 140.541 | 30.125 | 39.989 | 1.00 | 14.57 |
| | 1710 | CB | ALA | 229 | 140.320 | 29.069 | 41.059 | 1.00 | 11.49 |
| | 1711 | C | ALA | 229 | 140.572 | 31.513 | 40.619 | 1.00 | 22.21 |
| | 1712 | O | ALA | 229 | 139.606 | 32.272 | 40.505 | 1.00 | 26.82 |
| 20 | 1713 | N | LYS | 230 | 141.683 | 31.841 | 41.278 | 1.00 | 17.14 |
| | 1714 | CA | LYS | 230 | 141.836 | 33.136 | 41.933 | 1.00 | 13.72 |
| | 1715 | CB | LYS | 230 | 143.118 | 33.168 | 42.766 | 1.00 | 17.71 |
| | 1716 | CG | LYS | 230 | 143.067 | 32.332 | 44.030 | 1.00 | 14.07 |
| | 1717 | CD | LYS | 230 | 144.343 | 32.505 | 44.835 | 1.00 | 23.37 |
| 25 | 1718 | CE | LYS | 230 | 144.253 | 31.802 | 46.177 | 1.00 | 31.01 |
| | 1719 | NZ | LYS | 230 | 145.477 | 32.021 | 46.994 | 1.00 | 32.57 |
| | 1720 | C | LYS | 230 | 141.816 | 34.310 | 40.956 | 1.00 | 16.07 |
| | 1721 | O | LYS | 230 | 141.111 | 35.292 | 41.176 | 1.00 | 15.73 |
| | 1722 | N | LEU | 231 | 142.585 | 34.202 | 39.876 | 1.00 | 17.93 |
| 30 | 1723 | CA | LEU | 231 | 142.646 | 35.260 | 38.872 | 1.00 | 20.80 |
| | 1724 | CB | LEU | 231 | 143.653 | 34.911 | 37.775 | 1.00 | 18.38 |
| | 1725 | CG | LEU | 231 | 145.141 | 34.870 | 38.116 | 1.00 | 16.32 |
| | 1726 | CD1 | LEU | 231 | 145.920 | 34.518 | 36.863 | 1.00 | 14.82 |
| | 1727 | CD2 | LEU | 231 | 145.593 | 36.212 | 38.658 | 1.00 | 15.83 |
| 35 | 1728 | C | LEU | 231 | 141.287 | 35.506 | 38.233 | 1.00 | 24.81 |
| | 1729 | O | LEU | 231 | 140.828 | 36.647 | 38.151 | 1.00 | 28.14 |
| | 1730 | N | ASP | 232 | 140.648 | 34.427 | 37.790 | 1.00 | 28.52 |
| | 1731 | CA | ASP | 232 | 139.344 | 34.503 | 37.139 | 1.00 | 23.60 |
| | 1732 | CB | ASP | 232 | 138.878 | 33.104 | 36.736 | 1.00 | 20.22 |
| 40 | 1733 | CG | ASP | 232 | 137.737 | 33.137 | 35.742 | 1.00 | 29.93 |
| | 1734 | OD1 | ASP | 232 | 138.019 | 33.223 | 34.527 | 1.00 | 24.38 |
| | 1735 | OD2 | ASP | 232 | 136.564 | 33.079 | 36.174 | 1.00 | 26.36 |
| | 1736 | C | ASP | 232 | 138.300 | 35.170 | 38.032 | 1.00 | 20.67 |
| | 1737 | O | ASP | 232 | 137.622 | 36.111 | 37.612 | 1.00 | 15.86 |
| 45 | 1738 | N | PHE | 233 | 138.203 | 34.707 | 39.274 | 1.00 | 12.27 |
| | 1739 | CA | PHE | 233 | 137.244 | 35.260 | 40.219 | 1.00 | 12.59 |
| | 1740 | CB | PHE | 233 | 137.355 | 34.549 | 41.569 | 1.00 | 14.20 |
| | 1741 | CG | PHE | 233 | 136.243 | 34.887 | 42.524 | 1.00 | 30.75 |
| | 1742 | CD1 | PHE | 233 | 135.130 | 34.058 | 42.634 | 1.00 | 33.32 |
| 50 | 1743 | CD2 | PHE | 233 | 136.298 | 36.042 | 43.302 | 1.00 | 29.41 |

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|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 1744 | CE1 | PHE | 233 | 134.088 | 34.372 | 43.502 | 1.00 | 34.63 |
| | 1745 | CE2 | PHE | 233 | 135.263 | 36.365 | 44.172 | 1.00 | 31.81 |
| | 1746 | CZ | PHE | 233 | 134.155 | 35.528 | 44.272 | 1.00 | 32.38 |
| 5 | 1747 | C | PHE | 233 | 137.452 | 36.760 | 40.407 | 1.00 | 18.84 |
| | 1748 | O | PHE | 233 | 136.495 | 37.534 | 40.394 | 1.00 | 24.79 |
| | 1749 | N | ASN | 234 | 138.710 | 37.160 | 40.572 | 1.00 | 25.72 |
| | 1750 | CA | ASN | 234 | 139.057 | 38.563 | 40.770 | 1.00 | 20.56 |
| | 1751 | CB | ASN | 234 | 140.509 | 38.694 | 41.239 | 1.00 | 25.13 |
| | 1752 | CG | ASN | 234 | 140.702 | 38.249 | 42.683 | 1.00 | 30.65 |
| 10 | 1753 | OD1 | ASN | 234 | 139.738 | 37.996 | 43.406 | 1.00 | 21.26 |
| | 1754 | ND2 | ASN | 234 | 141.957 | 38.162 | 43.109 | 1.00 | 35.99 |
| | 1755 | C | ASN | 234 | 138.818 | 39.427 | 39.536 | 1.00 | 18.33 |
| | 1756 | O | ASN | 234 | 138.457 | 40.599 | 39.662 | 1.00 | 15.79 |
| | 1757 | N | LEU | 235 | 139.019 | 38.848 | 38.353 | 1.00 | 17.45 |
| 15 | 1758 | CA | LEU | 235 | 138.814 | 39.567 | 37.097 | 1.00 | 16.13 |
| | 1759 | CB | LEU | 235 | 139.402 | 38.789 | 35.920 | 1.00 | 14.09 |
| | 1760 | CG | LEU | 235 | 139.233 | 39.426 | 34.534 | 1.00 | 25.16 |
| | 1761 | CD1 | LEU | 235 | 139.947 | 40.774 | 34.472 | 1.00 | 16.26 |
| | 1762 | CD2 | LEU | 235 | 139.762 | 38.487 | 33.458 | 1.00 | 11.51 |
| 20 | 1763 | C | LEU | 235 | 137.329 | 39.812 | 36.866 | 1.00 | 23.53 |
| | 1764 | O | LEU | 235 | 136.929 | 40.918 | 36.502 | 1.00 | 30.18 |
| | 1765 | N | LEU | 236 | 136.517 | 38.773 | 37.065 | 1.00 | 26.97 |
| | 1766 | CA | LEU | 236 | 135.071 | 38.894 | 36.900 | 1.00 | 21.97 |
| | 1767 | CB | LEU | 236 | 134.375 | 37.538 | 37.041 | 1.00 | 22.99 |
| 25 | 1768 | CG | LEU | 236 | 134.550 | 36.506 | 35.931 | 1.00 | 24.74 |
| | 1769 | CD1 | LEU | 236 | 133.601 | 35.347 | 36.187 | 1.00 | 22.83 |
| | 1770 | CD2 | LEU | 236 | 134.259 | 37.133 | 34.579 | 1.00 | 26.05 |
| | 1771 | C | LEU | 236 | 134.511 | 39.858 | 37.935 | 1.00 | 15.40 |
| | 1772 | O | LEU | 236 | 133.581 | 40.602 | 37.646 | 1.00 | 21.06 |
| 30 | 1773 | N | GLN | 237 | 135.080 | 39.837 | 39.139 | 1.00 | 13.42 |
| | 1774 | CA | GLN | 237 | 134.645 | 40.721 | 40.217 | 1.00 | 14.55 |
| | 1775 | CB | GLN | 237 | 135.477 | 40.481 | 41.475 | 1.00 | 14.51 |
| | 1776 | CG | GLN | 237 | 135.051 | 41.318 | 42.671 | 1.00 | 12.72 |
| | 1777 | CD | GLN | 237 | 135.967 | 41.131 | 43.862 | 1.00 | 12.21 |
| 35 | 1778 | OE1 | GLN | 237 | 137.121 | 41.566 | 43.847 | 1.00 | 18.76 |
| | 1779 | NE2 | GLN | 237 | 135.460 | 40.483 | 44.900 | 1.00 | 4.88 |
| | 1780 | C | GLN | 237 | 134.760 | 42.180 | 39.788 | 1.00 | 22.23 |
| | 1781 | O | GLN | 237 | 133.950 | 43.011 | 40.192 | 1.00 | 28.74 |
| | 1782 | N | MET | 238 | 135.770 | 42.481 | 38.970 | 1.00 | 29.92 |
| 40 | 1783 | CA | MET | 238 | 135.985 | 43.833 | 38.458 | 1.00 | 23.66 |
| | 1784 | CB | MET | 238 | 137.275 | 43.906 | 37.638 | 1.00 | 25.72 |
| | 1785 | CG | MET | 238 | 138.552 | 43.791 | 38.454 | 1.00 | 26.38 |
| | 1786 | SD | MET | 238 | 140.030 | 43.684 | 37.408 | 1.00 | 30.42 |
| | 1787 | CE | MET | 238 | 141.233 | 43.058 | 38.580 | 1.00 | 23.83 |
| 45 | 1788 | C | MET | 238 | 134.801 | 44.227 | 37.584 | 1.00 | 20.92 |
| | 1789 | O | MET | 238 | 134.344 | 45.367 | 37.628 | 1.00 | 20.70 |
| | 1790 | N | LEU | 239 | 134.310 | 43.274 | 36.792 | 1.00 | 23.17 |
| | 1791 | CA | LEU | 239 | 133.159 | 43.509 | 35.920 | 1.00 | 21.15 |
| | 1792 | CB | LEU | 239 | 132.938 | 42.323 | 34.978 | 1.00 | 10.92 |
| 50 | 1793 | CG | LEU | 239 | 131.684 | 42.381 | 34.100 | 1.00 | 20.20 |

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|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 1794 | CD1 | LEU | 239 | 131.748 | 43.579 | 33.166 | 1.00 | 9.66 |
| | 1795 | CD2 | LEU | 239 | 131.541 | 41.089 | 33.309 | 1.00 | 10.55 |
| | 1796 | C | LEU | 239 | 131.908 | 43.732 | 36.764 | 1.00 | 14.68 |
| 5 | 1797 | O | LEU | 239 | 131.129 | 44.645 | 36.501 | 1.00 | 23.63 |
| | 1798 | N | HIS | 240 | 131.735 | 42.904 | 37.788 | 1.00 | 15.07 |
| | 1799 | CA | HIS | 240 | 130.587 | 43.015 | 38.680 | 1.00 | 19.33 |
| | 1800 | CB | HIS | 240 | 130.619 | 41.913 | 39.746 | 1.00 | 16.76 |
| | 1801 | CG | HIS | 240 | 130.661 | 40.525 | 39.185 | 1.00 | 12.10 |
| 10 | 1802 | CD2 | HIS | 240 | 130.296 | 40.039 | 37.973 | 1.00 | 12.51 |
| | 1803 | ND1 | HIS | 240 | 131.144 | 39.449 | 39.897 | 1.00 | 8.57 |
| | 1804 | CE1 | HIS | 240 | 131.077 | 38.362 | 39.150 | 1.00 | 16.05 |
| | 1805 | NE2 | HIS | 240 | 130.567 | 38.692 | 37.979 | 1.00 | 13.30 |
| | 1806 | C | HIS | 240 | 130.610 | 44.383 | 39.344 | 1.00 | 21.46 |
| 15 | 1807 | O | HIS | 240 | 129.572 | 45.034 | 39.481 | 1.00 | 28.61 |
| | 1808 | N | LYS | 241 | 131.809 | 44.819 | 39.728 | 1.00 | 24.98 |
| | 1809 | CA | LYS | 241 | 132.008 | 46.118 | 40.364 | 1.00 | 19.85 |
| | 1810 | CB | LYS | 241 | 133.469 | 46.281 | 40.782 | 1.00 | 18.41 |
| | 1811 | CG | LYS | 241 | 133.855 | 45.556 | 42.057 | 1.00 | 18.41 |
| 20 | 1812 | CD | LYS | 241 | 135.348 | 45.688 | 42.297 | 1.00 | 29.39 |
| | 1813 | CE | LYS | 241 | 135.667 | 45.861 | 43.769 | 1.00 | 43.69 |
| | 1814 | NZ | LYS | 241 | 137.131 | 45.987 | 43.991 | 1.00 | 46.04 |
| | 1815 | C | LYS | 241 | 131.604 | 47.252 | 39.419 | 1.00 | 23.69 |
| | 1816 | O | LYS | 241 | 130.983 | 48.229 | 39.845 | 1.00 | 14.81 |
| 25 | 1817 | N | GLN | 242 | 131.954 | 47.107 | 38.140 | 1.00 | 20.70 |
| | 1818 | CA | GLN | 242 | 131.615 | 48.099 | 37.120 | 1.00 | 28.94 |
| | 1819 | CB | GLN | 242 | 132.262 | 47.748 | 35.775 | 1.00 | 29.06 |
| | 1820 | CG | GLN | 242 | 133.775 | 47.862 | 35.748 | 1.00 | 39.14 |
| | 1821 | CD | GLN | 242 | 134.359 | 47.517 | 34.392 | 1.00 | 42.97 |
| 30 | 1822 | OE1 | GLN | 242 | 134.324 | 46.363 | 33.962 | 1.00 | 48.36 |
| | 1823 | NE2 | GLN | 242 | 134.904 | 48.519 | 33.710 | 1.00 | 39.66 |
| | 1824 | C | GLN | 242 | 130.103 | 48.163 | 36.943 | 1.00 | 33.40 |
| | 1825 | O | GLN | 242 | 129.514 | 49.246 | 36.938 | 1.00 | 40.80 |
| | 1826 | N | GLU | 243 | 129.487 | 46.992 | 36.807 | 1.00 | 33.80 |
| 35 | 1827 | CA | GLU | 243 | 128.044 | 46.884 | 36.631 | 1.00 | 22.54 |
| | 1828 | CB | GLU | 243 | 127.647 | 45.420 | 36.466 | 1.00 | 15.53 |
| | 1829 | CG | GLU | 243 | 128.204 | 44.778 | 35.210 | 1.00 | 15.70 |
| | 1830 | CD | GLU | 243 | 127.938 | 43.290 | 35.137 | 1.00 | 18.78 |
| | 1831 | OE1 | GLU | 243 | 127.639 | 42.675 | 36.178 | 1.00 | 18.01 |
| 40 | 1832 | OE2 | GLU | 243 | 128.040 | 42.727 | 34.032 | 1.00 | 15.89 |
| | 1833 | C | GLU | 243 | 127.290 | 47.495 | 37.806 | 1.00 | 20.49 |
| | 1834 | O | GLU | 243 | 126.351 | 48.266 | 37.611 | 1.00 | 18.81 |
| | 1835 | N | LEU | 244 | 127.715 | 47.159 | 39.022 | 1.00 | 12.97 |
| | 1836 | CA | LEU | 244 | 127.079 | 47.675 | 40.231 | 1.00 | 15.01 |
| 45 | 1837 | CB | LEU | 244 | 127.676 | 46.999 | 41.467 | 1.00 | 12.34 |
| | 1838 | CG | LEU | 244 | 127.144 | 47.436 | 42.832 | 1.00 | 12.62 |
| | 1839 | CD1 | LEU | 244 | 125.628 | 47.332 | 42.881 | 1.00 | 24.09 |
| | 1840 | CD2 | LEU | 244 | 127.780 | 46.582 | 43.908 | 1.00 | 9.05 |
| | 1841 | C | LEU | 244 | 127.213 | 49.191 | 40.335 | 1.00 | 22.78 |
| | 1842 | O | LEU | 244 | 126.328 | 49.868 | 40.863 | 1.00 | 27.46 |
| 50 | 1843 | N | ALA | 245 | 128.325 | 49.725 | 39.838 | 1.00 | 31.72 |

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|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 1844 | CA | ALA | 245 | 128.560 | 51.167 | 39.856 | 1.00 | 30.71 |
| | 1845 | CB | ALA | 245 | 129.998 | 51.476 | 39.466 | 1.00 | 26.12 |
| | 1846 | C | ALA | 245 | 127.589 | 51.860 | 38.893 | 1.00 | 29.98 |
| | 1847 | O | ALA | 245 | 127.005 | 52.887 | 39.226 | 1.00 | 32.44 |
| 5 | 1848 | N | GLN | 246 | 127.410 | 51.256 | 37.718 | 1.00 | 29.03 |
| | 1849 | CA | GLN | 246 | 126.528 | 51.754 | 36.668 | 1.00 | 31.14 |
| | 1850 | CB | GLN | 246 | 126.689 | 50.868 | 35.430 | 1.00 | 31.92 |
| | 1851 | CG | GLN | 246 | 125.845 | 51.244 | 34.232 | 1.00 | 41.36 |
| | 1852 | CD | GLN | 246 | 125.970 | 50.235 | 33.109 | 1.00 | 48.09 |
| 10 | 1853 | OE1 | GLN | 246 | 127.023 | 49.627 | 32.919 | 1.00 | 49.29 |
| | 1854 | NE2 | GLN | 246 | 124.887 | 50.043 | 32.361 | 1.00 | 55.11 |
| | 1855 | C | GLN | 246 | 125.074 | 51.762 | 37.119 | 1.00 | 34.84 |
| | 1856 | O | GLN | 246 | 124.297 | 52.637 | 36.732 | 1.00 | 42.31 |
| | 1857 | N | VAL | 247 | 124.719 | 50.762 | 37.921 | 1.00 | 39.27 |
| 15 | 1858 | CA | VAL | 247 | 123.360 | 50.631 | 38.441 | 1.00 | 38.03 |
| | 1859 | CB | VAL | 247 | 123.069 | 49.138 | 38.742 | 1.00 | 38.04 |
| | 1860 | CG1 | VAL | 247 | 122.330 | 48.954 | 40.059 | 1.00 | 39.31 |
| | 1861 | CG2 | VAL | 247 | 122.270 | 48.526 | 37.603 | 1.00 | 37.60 |
| | 1862 | C | VAL | 247 | 123.144 | 51.507 | 39.667 | 1.00 | 37.49 |
| 20 | 1863 | O | VAL | 247 | 122.012 | 51.862 | 39.998 | 1.00 | 33.11 |
| | 1864 | N | SER | 248 | 124.231 | 51.871 | 40.340 | 1.00 | 39.80 |
| | 1865 | CA | SER | 248 | 124.173 | 52.736 | 41.515 | 1.00 | 43.54 |
| | 1866 | CB | SER | 248 | 125.456 | 52.604 | 42.352 | 1.00 | 41.35 |
| | 1867 | OG | SER | 248 | 125.482 | 51.368 | 43.057 | 1.00 | 23.81 |
| 25 | 1868 | C | SER | 248 | 123.963 | 54.195 | 41.093 | 1.00 | 41.56 |
| | 1869 | O | SER | 248 | 123.288 | 54.976 | 41.783 | 1.00 | 39.28 |
| | 1870 | N | ARG | 249 | 124.591 | 54.559 | 39.974 | 1.00 | 40.01 |
| | 1871 | CA | ARG | 249 | 124.467 | 55.901 | 39.421 | 1.00 | 47.97 |
| | 1872 | CB | ARG | 249 | 125.475 | 56.127 | 38.290 | 1.00 | 51.84 |
| 30 | 1873 | CG | ARG | 249 | 126.912 | 56.292 | 38.747 | 1.00 | 62.62 |
| | 1874 | CD | ARG | 249 | 127.836 | 56.501 | 37.563 | 1.00 | 69.45 |
| | 1875 | NE | ARG | 249 | 129.065 | 55.731 | 37.713 | 1.00 | 78.07 |
| | 1876 | CZ | ARG | 249 | 129.491 | 54.824 | 36.840 | 1.00 | 81.11 |
| | 1877 | NH1 | ARG | 249 | 128.795 | 54.570 | 35.737 | 1.00 | 75.69 |
| 35 | 1878 | NH2 | ARG | 249 | 130.602 | 54.145 | 37.087 | 1.00 | 86.20 |
| | 1879 | C | ARG | 249 | 123.051 | 56.058 | 38.890 | 1.00 | 43.68 |
| | 1880 | O | ARG | 249 | 122.402 | 57.072 | 39.127 | 1.00 | 45.81 |
| | 1881 | N | TRP | 250 | 122.588 | 55.030 | 38.183 | 1.00 | 38.57 |
| | 1882 | CA | TRP | 250 | 121.247 | 55.000 | 37.613 | 1.00 | 34.46 |
| 40 | 1883 | CB | TRP | 250 | 121.060 | 53.682 | 36.851 | 1.00 | 37.42 |
| | 1884 | CG | TRP | 250 | 119.635 | 53.325 | 36.531 | 1.00 | 37.50 |
| | 1885 | CD2 | TRP | 250 | 118.745 | 52.545 | 37.341 | 1.00 | 32.98 |
| | 1886 | CE2 | TRP | 250 | 117.516 | 52.464 | 36.652 | 1.00 | 39.28 |
| | 1887 | CE3 | TRP | 250 | 118.867 | 51.909 | 38.585 | 1.00 | 32.90 |
| 45 | 1888 | CD1 | TRP | 250 | 118.931 | 53.672 | 35.413 | 1.00 | 28.29 |
| | 1889 | NE1 | TRP | 250 | 117.658 | 53.159 | 35.479 | 1.00 | 36.07 |
| | 1890 | CZ2 | TRP | 250 | 116.411 | 51.771 | 37.167 | 1.00 | 40.28 |
| | 1891 | CZ3 | TRP | 250 | 117.770 | 51.221 | 39.098 | 1.00 | 33.00 |
| | 1892 | CH2 | TRP | 250 | 116.557 | 51.159 | 38.388 | 1.00 | 34.10 |
| 50 | 1893 | C | TRP | 250 | 120.215 | 55.131 | 38.731 | 1.00 | 31.76 |

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|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 1894 | O | TRP | 250 | 119.207 | 55.820 | 38.583 | 1.00 | 38.62 |
| | 1895 | N | TRP | 251 | 120.499 | 54.493 | 39.861 | 1.00 | 29.34 |
| | 1896 | CA | TRP | 251 | 119.611 | 54.513 | 41.017 | 1.00 | 28.23 |
| | 1897 | CB | TRP | 251 | 120.041 | 53.431 | 42.003 | 1.00 | 24.43 |
| 5 | 1898 | CG | TRP | 251 | 119.164 | 53.309 | 43.196 | 1.00 | 27.54 |
| | 1899 | CD2 | TRP | 251 | 117.813 | 52.824 | 43.224 | 1.00 | 28.47 |
| | 1900 | CE2 | TRP | 251 | 117.394 | 52.848 | 44.576 | 1.00 | 30.61 |
| | 1901 | CE3 | TRP | 251 | 116.921 | 52.373 | 42.246 | 1.00 | 22.56 |
| 10 | 1902 | CD1 | TRP | 251 | 119.493 | 53.603 | 44.486 | 1.00 | 29.85 |
| | 1903 | NE1 | TRP | 251 | 118.439 | 53.327 | 45.321 | 1.00 | 28.21 |
| | 1904 | CZ2 | TRP | 251 | 116.117 | 52.434 | 44.974 | 1.00 | 27.80 |
| | 1905 | CZ3 | TRP | 251 | 115.646 | 51.959 | 42.641 | 1.00 | 16.40 |
| | 1906 | CH2 | TRP | 251 | 115.261 | 51.995 | 43.993 | 1.00 | 23.32 |
| | 1907 | C | TRP | 251 | 119.575 | 55.877 | 41.703 | 1.00 | 37.98 |
| 15 | 1908 | O | TRP | 251 | 118.564 | 56.243 | 42.309 | 1.00 | 45.16 |
| | 1909 | N | LYS | 252 | 120.685 | 56.610 | 41.636 | 1.00 | 42.00 |
| | 1910 | CA | LYS | 252 | 120.758 | 57.938 | 42.238 | 1.00 | 42.12 |
| | 1911 | CB | LYS | 252 | 122.198 | 58.328 | 42.551 | 1.00 | 47.95 |
| | 1912 | CG | LYS | 252 | 122.598 | 58.028 | 43.975 | 1.00 | 54.42 |
| 20 | 1913 | CD | LYS | 252 | 123.720 | 58.943 | 44.418 | 1.00 | 63.61 |
| | 1914 | CE | LYS | 252 | 123.889 | 58.896 | 45.923 | 1.00 | 76.47 |
| | 1915 | NZ | LYS | 252 | 124.827 | 59.944 | 46.407 | 1.00 | 82.00 |
| | 1916 | C | LYS | 252 | 120.113 | 58.992 | 41.348 | 1.00 | 43.32 |
| | 1917 | O | LYS | 252 | 119.528 | 59.955 | 41.845 | 1.00 | 40.24 |
| 25 | 1918 | N | ASP | 253 | 120.220 | 58.802 | 40.033 | 1.00 | 41.81 |
| | 1919 | CA | ASP | 253 | 119.621 | 59.715 | 39.061 | 1.00 | 42.20 |
| | 1920 | CB | ASP | 253 | 119.991 | 59.305 | 37.632 | 1.00 | 46.23 |
| | 1921 | CG | ASP | 253 | 121.475 | 59.448 | 37.340 | 1.00 | 56.62 |
| | 1922 | OD1 | ASP | 253 | 122.222 | 59.973 | 38.197 | 1.00 | 59.66 |
| 30 | 1923 | OD2 | ASP | 253 | 121.896 | 59.029 | 36.240 | 1.00 | 59.43 |
| | 1924 | C | ASP | 253 | 118.100 | 59.701 | 39.208 | 1.00 | 46.95 |
| | 1925 | O | ASP | 253 | 117.404 | 60.508 | 38.597 | 1.00 | 47.82 |
| | 1926 | N | LEU | 254 | 117.600 | 58.743 | 39.987 | 1.00 | 50.43 |
| | 1927 | CA | LEU | 254 | 116.172 | 58.596 | 40.253 | 1.00 | 52.57 |
| 35 | 1928 | CB | LEU | 254 | 115.777 | 57.116 | 40.236 | 1.00 | 51.09 |
| | 1929 | CG | LEU | 254 | 116.036 | 56.357 | 38.930 | 1.00 | 52.73 |
| | 1930 | CD1 | LEU | 254 | 115.673 | 54.894 | 39.102 | 1.00 | 50.16 |
| | 1931 | CD2 | LEU | 254 | 115.244 | 56.974 | 37.788 | 1.00 | 48.48 |
| | 1932 | C | LEU | 254 | 115.867 | 59.205 | 41.619 | 1.00 | 50.66 |
| 40 | 1933 | O | LEU | 254 | 114.780 | 59.735 | 41.848 | 1.00 | 48.89 |
| | 1934 | N | ASP | 255 | 116.838 | 59.099 | 42.522 | 1.00 | 54.73 |
| | 1935 | CA | ASP | 255 | 116.750 | 59.641 | 43.875 | 1.00 | 59.42 |
| | 1936 | CB | ASP | 255 | 116.930 | 61.167 | 43.829 | 1.00 | 63.16 |
| | 1937 | CG | ASP | 255 | 117.232 | 61.774 | 45.193 | 1.00 | 70.47 |
| 45 | 1938 | OD1 | ASP | 255 | 117.674 | 61.045 | 46.110 | 1.00 | 70.14 |
| | 1939 | OD2 | ASP | 255 | 117.030 | 62.997 | 45.344 | 1.00 | 79.11 |
| | 1940 | C | ASP | 255 | 115.476 | 59.260 | 44.640 | 1.00 | 56.10 |
| | 1941 | O | ASP | 255 | 114.834 | 60.106 | 45.263 | 1.00 | 54.97 |
| | 1942 | N | PHE | 256 | 115.127 | 57.977 | 44.602 | 1.00 | 55.78 |
| 50 | 1943 | CA | PHE | 256 | 113.946 | 57.486 | 45.308 | 1.00 | 55.28 |

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|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 1944 | CB | PHE | 256 | 113.556 | 56.093 | 44.808 | 1.00 | 51.79 |
| | 1945 | CG | PHE | 256 | 113.024 | 56.079 | 43.407 | 1.00 | 52.55 |
| | 1946 | CD1 | PHE | 256 | 113.356 | 55.051 | 42.537 | 1.00 | 55.14 |
| | 1947 | CD2 | PHE | 256 | 112.186 | 57.091 | 42.955 | 1.00 | 58.21 |
| 5 | 1948 | CE1 | PHE | 256 | 112.862 | 55.028 | 41.236 | 1.00 | 57.90 |
| | 1949 | CE2 | PHE | 256 | 111.687 | 57.077 | 41.656 | 1.00 | 60.53 |
| | 1950 | CZ | PHE | 256 | 112.026 | 56.042 | 40.796 | 1.00 | 57.76 |
| | 1951 | C | PHE | 256 | 114.199 | 57.438 | 46.812 | 1.00 | 60.70 |
| | 1952 | O | PHE | 256 | 113.292 | 57.162 | 47.596 | 1.00 | 62.84 |
| 10 | 1953 | N | VAL | 257 | 115.442 | 57.704 | 47.203 | 1.00 | 64.41 |
| | 1954 | CA | VAL | 257 | 115.834 | 57.697 | 48.606 | 1.00 | 64.01 |
| | 1955 | CB | VAL | 257 | 117.373 | 57.799 | 48.757 | 1.00 | 62.36 |
| | 1956 | CG1 | VAL | 257 | 117.789 | 57.482 | 50.187 | 1.00 | 60.29 |
| | 1957 | CG2 | VAL | 257 | 118.068 | 56.864 | 47.774 | 1.00 | 58.27 |
| 15 | 1958 | C | VAL | 257 | 115.179 | 58.870 | 49.333 | 1.00 | 65.72 |
| | 1959 | O | VAL | 257 | 114.849 | 58.771 | 50.517 | 1.00 | 64.55 |
| | 1960 | N | THR | 258 | 114.977 | 59.971 | 48.609 | 1.00 | 66.40 |
| | 1961 | CA | THR | 258 | 114.364 | 61.171 | 49.175 | 1.00 | 65.40 |
| | 1962 | CB | THR | 258 | 115.200 | 62.437 | 48.870 | 1.00 | 65.98 |
| 20 | 1963 | OG1 | THR | 258 | 115.282 | 62.633 | 47.453 | 1.00 | 65.25 |
| | 1964 | CG2 | THR | 258 | 116.608 | 62.302 | 49.442 | 1.00 | 64.28 |
| | 1965 | C | THR | 258 | 112.919 | 61.399 | 48.716 | 1.00 | 62.28 |
| | 1966 | O | THR | 258 | 112.066 | 61.769 | 49.524 | 1.00 | 62.30 |
| | 1967 | N | THR | 259 | 112.649 | 61.182 | 47.428 | 1.00 | 58.00 |
| 25 | 1968 | CA | THR | 259 | 111.303 | 61.372 | 46.879 | 1.00 | 53.45 |
| | 1969 | CB | THR | 259 | 111.300 | 61.402 | 45.332 | 1.00 | 48.24 |
| | 1970 | OG1 | THR | 259 | 111.730 | 60.136 | 44.818 | 1.00 | 47.10 |
| | 1971 | CG2 | THR | 259 | 112.221 | 62.496 | 44.817 | 1.00 | 44.78 |
| | 1972 | C | THR | 259 | 110.320 | 60.303 | 47.358 | 1.00 | 54.85 |
| 30 | 1973 | O | THR | 259 | 109.147 | 60.593 | 47.593 | 1.00 | 58.40 |
| | 1974 | N | LEU | 260 | 110.802 | 59.069 | 47.492 | 1.00 | 54.85 |
| | 1975 | CA | LEU | 260 | 109.977 | 57.952 | 47.958 | 1.00 | 57.07 |
| | 1976 | CB | LEU | 260 | 109.811 | 56.907 | 46.845 | 1.00 | 54.53 |
| | 1977 | CG | LEU | 260 | 109.191 | 57.346 | 45.511 | 1.00 | 54.02 |
| 35 | 1978 | CD1 | LEU | 260 | 109.216 | 56.192 | 44.523 | 1.00 | 47.30 |
| | 1979 | CD2 | LEU | 260 | 107.765 | 57.838 | 45.715 | 1.00 | 53.62 |
| | 1980 | C | LEU | 260 | 110.655 | 57.326 | 49.183 | 1.00 | 59.06 |
| | 1981 | O | LEU | 260 | 111.135 | 56.190 | 49.132 | 1.00 | 61.18 |
| | 1982 | N | PRO | 261 | 110.672 | 58.057 | 50.314 | 1.00 | 59.80 |
| 40 | 1983 | CD | PRO | 261 | 110.004 | 59.362 | 50.474 | 1.00 | 57.03 |
| | 1984 | CA | PRO | 261 | 111.281 | 57.634 | 51.582 | 1.00 | 60.02 |
| | 1985 | CB | PRO | 261 | 111.144 | 58.883 | 52.452 | 1.00 | 59.64 |
| | 1986 | CG | PRO | 261 | 109.865 | 59.476 | 51.972 | 1.00 | 61.83 |
| | 1987 | C | PRO | 261 | 110.685 | 56.401 | 52.265 | 1.00 | 56.67 |
| 45 | 1988 | O | PRO | 261 | 111.317 | 55.811 | 53.143 | 1.00 | 54.94 |
| | 1989 | N | TYR | 262 | 109.475 | 56.019 | 51.869 | 1.00 | 55.28 |
| | 1990 | CA | TYR | 262 | 108.813 | 54.855 | 52.455 | 1.00 | 52.74 |
| | 1991 | CB | TYR | 262 | 107.309 | 54.898 | 52.167 | 1.00 | 46.52 |
| | 1992 | CG | TYR | 262 | 106.954 | 54.869 | 50.695 | 1.00 | 38.58 |
| 50 | 1993 | CD1 | TYR | 262 | 106.624 | 53.671 | 50.062 | 1.00 | 30.09 |

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|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 1994 | CE1 | TYR | 262 | 106.295 | 53.636 | 48.711 | 1.00 | 29.27 |
| | 1995 | CD2 | TYR | 262 | 106.944 | 56.039 | 49.936 | 1.00 | 34.60 |
| | 1996 | CE2 | TYR | 262 | 106.614 | 56.015 | 48.581 | 1.00 | 37.08 |
| 5 | 1997 | CZ | TYR | 262 | 106.290 | 54.809 | 47.974 | 1.00 | 32.64 |
| | 1998 | OH | TYR | 262 | 105.961 | 54.776 | 46.635 | 1.00 | 17.43 |
| | 1999 | C | TYR | 262 | 109.398 | 53.534 | 51.956 | 1.00 | 52.07 |
| | 2000 | O | TYR | 262 | 109.356 | 52.522 | 52.658 | 1.00 | 51.95 |
| | 2001 | N | ALA | 263 | 109.957 | 53.565 | 50.748 | 1.00 | 48.22 |
| 10 | 2002 | CA | ALA | 263 | 110.545 | 52.386 | 50.120 | 1.00 | 49.01 |
| | 2003 | CB | ALA | 263 | 110.701 | 52.627 | 48.623 | 1.00 | 44.24 |
| | 2004 | C | ALA | 263 | 111.879 | 51.943 | 50.723 | 1.00 | 52.04 |
| | 2005 | O | ALA | 263 | 112.458 | 52.631 | 51.567 | 1.00 | 52.30 |
| | 2006 | N | ARG | 264 | 112.333 | 50.766 | 50.297 | 1.00 | 53.43 |
| 15 | 2007 | CA | ARG | 264 | 113.592 | 50.196 | 50.752 | 1.00 | 48.17 |
| | 2008 | CB | ARG | 264 | 113.499 | 48.670 | 50.889 | 1.00 | 40.34 |
| | 2009 | CG | ARG | 264 | 112.624 | 48.166 | 52.030 | 1.00 | 43.53 |
| | 2010 | CD | ARG | 264 | 112.450 | 46.639 | 51.996 | 1.00 | 35.92 |
| | 2011 | NE | ARG | 264 | 111.772 | 46.200 | 50.774 | 1.00 | 44.75 |
| 20 | 2012 | CZ | ARG | 264 | 110.964 | 45.144 | 50.679 | 1.00 | 49.82 |
| | 2013 | NH1 | ARG | 264 | 110.714 | 44.385 | 51.738 | 1.00 | 51.07 |
| | 2014 | NH2 | ARG | 264 | 110.385 | 44.857 | 49.518 | 1.00 | 37.04 |
| | 2015 | C | ARG | 264 | 114.676 | 50.512 | 49.742 | 1.00 | 49.03 |
| | 2016 | O | ARG | 264 | 114.453 | 50.444 | 48.527 | 1.00 | 47.55 |
| 25 | 2017 | N | ASP | 265 | 115.848 | 50.870 | 50.252 | 1.00 | 50.80 |
| | 2018 | CA | ASP | 265 | 116.987 | 51.164 | 49.392 | 1.00 | 51.29 |
| | 2019 | CB | ASP | 265 | 117.728 | 52.418 | 49.877 | 1.00 | 52.76 |
| | 2020 | CG | ASP | 265 | 118.690 | 52.955 | 48.843 | 1.00 | 54.37 |
| | 2021 | OD1 | ASP | 265 | 118.782 | 52.363 | 47.747 | 1.00 | 50.00 |
| 30 | 2022 | OD2 | ASP | 265 | 119.358 | 53.972 | 49.120 | 1.00 | 60.30 |
| | 2023 | C | ASP | 265 | 117.903 | 49.933 | 49.419 | 1.00 | 45.08 |
| | 2024 | O | ASP | 265 | 118.824 | 49.846 | 50.238 | 1.00 | 39.53 |
| | 2025 | N | ARG | 266 | 117.614 | 48.973 | 48.541 | 1.00 | 41.67 |
| | 2026 | CA | ARG | 266 | 118.377 | 47.732 | 48.462 | 1.00 | 37.99 |
| 35 | 2027 | CB | ARG | 266 | 117.528 | 46.574 | 48.983 | 1.00 | 38.78 |
| | 2028 | CG | ARG | 266 | 116.957 | 46.771 | 50.372 | 1.00 | 29.99 |
| | 2029 | CD | ARG | 266 | 118.028 | 46.593 | 51.418 | 1.00 | 37.48 |
| | 2030 | NE | ARG | 266 | 117.503 | 46.781 | 52.764 | 1.00 | 38.27 |
| | 2031 | CZ | ARG | 266 | 117.416 | 47.958 | 53.376 | 1.00 | 45.66 |
| 40 | 2032 | NH1 | ARG | 266 | 117.822 | 49.066 | 52.763 | 1.00 | 38.28 |
| | 2033 | NH2 | ARG | 266 | 116.920 | 48.027 | 54.603 | 1.00 | 42.90 |
| | 2034 | C | ARG | 266 | 118.826 | 47.429 | 47.034 | 1.00 | 33.86 |
| | 2035 | O | ARG | 266 | 118.671 | 46.306 | 46.542 | 1.00 | 40.81 |
| | 2036 | N | VAL | 267 | 119.392 | 48.431 | 46.371 | 1.00 | 25.69 |
| 45 | 2037 | CA | VAL | 267 | 119.845 | 48.257 | 45.000 | 1.00 | 20.97 |
| | 2038 | CB | VAL | 267 | 120.143 | 49.611 | 44.326 | 1.00 | 21.69 |
| | 2039 | CG1 | VAL | 267 | 121.384 | 50.264 | 44.933 | 1.00 | 20.36 |
| | 2040 | CG2 | VAL | 267 | 120.292 | 49.420 | 42.828 | 1.00 | 8.30 |
| | 2041 | C | VAL | 267 | 121.058 | 47.333 | 44.913 | 1.00 | 27.40 |
| 50 | 2042 | O | VAL | 267 | 121.231 | 46.616 | 43.926 | 1.00 | 36.12 |
| | 2043 | N | VAL | 268 | 121.889 | 47.347 | 45.952 | 1.00 | 30.76 |

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|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 2044 | CA | VAL | 268 | 123.080 | 46.503 | 46.008 | 1.00 | 32.68 |
| | 2045 | CB | VAL | 268 | 123.998 | 46.904 | 47.190 | 1.00 | 35.53 |
| | 2046 | CG1 | VAL | 268 | 125.220 | 46.001 | 47.245 | 1.00 | 32.24 |
| | 2047 | CG2 | VAL | 268 | 124.420 | 48.355 | 47.058 | 1.00 | 33.69 |
| 5 | 2048 | C | VAL | 268 | 122.623 | 45.058 | 46.196 | 1.00 | 29.06 |
| | 2049 | O | VAL | 268 | 123.119 | 44.144 | 45.533 | 1.00 | 25.58 |
| | 2050 | N | GLU | 269 | 121.662 | 44.878 | 47.100 | 1.00 | 24.94 |
| | 2051 | CA | GLU | 269 | 121.087 | 43.573 | 47.406 | 1.00 | 22.59 |
| | 2052 | CB | GLU | 269 | 120.083 | 43.692 | 48.558 | 1.00 | 16.86 |
| 10 | 2053 | CG | GLU | 269 | 120.705 | 43.939 | 49.942 | 1.00 | 22.84 |
| | 2054 | CD | GLU | 269 | 121.136 | 45.385 | 50.200 | 1.00 | 25.18 |
| | 2055 | OE1 | GLU | 269 | 121.417 | 45.713 | 51.374 | 1.00 | 24.26 |
| | 2056 | OE2 | GLU | 269 | 121.194 | 46.198 | 49.255 | 1.00 | 23.69 |
| | 2057 | C | GLU | 269 | 120.404 | 43.001 | 46.167 | 1.00 | 21.52 |
| 15 | 2058 | O | GLU | 269 | 120.423 | 41.789 | 45.941 | 1.00 | 22.99 |
| | 2059 | N | CYS | 270 | 119.814 | 43.885 | 45.365 | 1.00 | 16.93 |
| | 2060 | CA | CYS | 270 | 119.144 | 43.487 | 44.133 | 1.00 | 15.61 |
| | 2061 | CB | CYS | 270 | 118.305 | 44.637 | 43.577 | 1.00 | 14.26 |
| | 2062 | SG | CYS | 270 | 116.923 | 45.097 | 44.637 | 1.00 | 24.62 |
| 20 | 2063 | C | CYS | 270 | 120.191 | 43.065 | 43.117 | 1.00 | 19.83 |
| | 2064 | O | CYS | 270 | 119.922 | 42.239 | 42.245 | 1.00 | 25.94 |
| | 2065 | N | TYR | 271 | 121.382 | 43.648 | 43.220 | 1.00 | 25.82 |
| | 2066 | CA | TYR | 271 | 122.464 | 43.290 | 42.315 | 1.00 | 22.31 |
| | 2067 | CB | TYR | 271 | 123.616 | 44.296 | 42.366 | 1.00 | 15.29 |
| 25 | 2068 | CG | TYR | 271 | 124.715 | 43.914 | 41.408 | 1.00 | 11.26 |
| | 2069 | CD1 | TYR | 271 | 124.592 | 44.174 | 40.043 | 1.00 | 9.23 |
| | 2070 | CE1 | TYR | 271 | 125.534 | 43.705 | 39.135 | 1.00 | 12.75 |
| | 2071 | CD2 | TYR | 271 | 125.821 | 43.184 | 41.844 | 1.00 | 6.39 |
| | 2072 | CE2 | TYR | 271 | 126.767 | 42.709 | 40.946 | 1.00 | 6.94 |
| 30 | 2073 | CZ | TYR | 271 | 126.615 | 42.970 | 39.594 | 1.00 | 11.07 |
| | 2074 | OH | TYR | 271 | 127.525 | 42.467 | 38.702 | 1.00 | 9.47 |
| | 2075 | C | TYR | 271 | 122.973 | 41.904 | 42.692 | 1.00 | 23.07 |
| | 2076 | O | TYR | 271 | 123.318 | 41.104 | 41.820 | 1.00 | 22.92 |
| | 2077 | N | PHE | 272 | 123.037 | 41.639 | 43.997 | 1.00 | 17.89 |
| 35 | 2078 | CA | PHE | 272 | 123.484 | 40.344 | 44.500 | 1.00 | 17.87 |
| | 2079 | CB | PHE | 272 | 123.481 | 40.329 | 46.033 | 1.00 | 20.14 |
| | 2080 | CG | PHE | 272 | 123.722 | 38.967 | 46.625 | 1.00 | 18.24 |
| | 2081 | CD1 | PHE | 272 | 124.998 | 38.409 | 46.631 | 1.00 | 20.70 |
| | 2082 | CD2 | PHE | 272 | 122.669 | 38.232 | 47.160 | 1.00 | 19.50 |
| 40 | 2083 | CE1 | PHE | 272 | 125.219 | 37.139 | 47.159 | 1.00 | 15.25 |
| | 2084 | CE2 | PHE | 272 | 122.881 | 36.961 | 47.690 | 1.00 | 17.71 |
| | 2085 | CZ | PHE | 272 | 124.159 | 36.414 | 47.689 | 1.00 | 12.72 |
| | 2086 | C | PHE | 272 | 122.540 | 39.273 | 43.972 | 1.00 | 20.61 |
| | 2087 | O | PHE | 272 | 122.974 | 38.200 | 43.550 | 1.00 | 26.50 |
| 45 | 2088 | N | TRP | 273 | 121.248 | 39.594 | 43.982 | 1.00 | 24.31 |
| | 2089 | CA | TRP | 273 | 120.203 | 38.695 | 43.506 | 1.00 | 20.50 |
| | 2090 | CB | TRP | 273 | 118.831 | 39.335 | 43.724 | 1.00 | 22.07 |
| | 2091 | CG | TRP | 273 | 117.820 | 38.395 | 44.280 | 1.00 | 22.11 |
| | 2092 | CD2 | TRP | 273 | 117.499 | 38.205 | 45.661 | 1.00 | 17.16 |
| 50 | 2093 | CE2 | TRP | 273 | 116.513 | 37.193 | 45.726 | 1.00 | 18.77 |

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|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 2094 | CE3 | TRP | 273 | 117.949 | 38.789 | 46.851 | 1.00 | 16.10 |
| | 2095 | CD1 | TRP | 273 | 117.036 | 37.522 | 43.580 | 1.00 | 22.90 |
| | 2096 | NE1 | TRP | 273 | 116.250 | 36.794 | 44.442 | 1.00 | 15.33 |
| | 2097 | CZ2 | TRP | 273 | 115.969 | 36.750 | 46.938 | 1.00 | 8.52 |
| 5 | 2098 | CZ3 | TRP | 273 | 117.408 | 38.351 | 48.057 | 1.00 | 19.38 |
| | 2099 | CH2 | TRP | 273 | 116.428 | 37.339 | 48.088 | 1.00 | 25.09 |
| | 2100 | C | TRP | 273 | 120.401 | 38.389 | 42.024 | 1.00 | 19.25 |
| | 2101 | O | TRP | 273 | 120.291 | 37.239 | 41.596 | 1.00 | 26.32 |
| | 2102 | N | ALA | 274 | 120.705 | 39.424 | 41.247 | 1.00 | 15.42 |
| 10 | 2103 | CA | ALA | 274 | 120.925 | 39.267 | 39.815 | 1.00 | 17.00 |
| | 2104 | CB | ALA | 274 | 120.927 | 40.622 | 39.138 | 1.00 | 8.15 |
| | 2105 | C | ALA | 274 | 122.240 | 38.538 | 39.553 | 1.00 | 21.87 |
| | 2106 | O | ALA | 274 | 122.394 | 37.858 | 38.535 | 1.00 | 24.79 |
| | 2107 | N | LEU | 275 | 123.188 | 38.694 | 40.474 | 1.00 | 18.76 |
| 15 | 2108 | CA | LEU | 275 | 124.487 | 38.045 | 40.354 | 1.00 | 20.76 |
| | 2109 | CB | LEU | 275 | 125.505 | 38.712 | 41.281 | 1.00 | 15.67 |
| | 2110 | CG | LEU | 275 | 126.937 | 38.176 | 41.221 | 1.00 | 6.06 |
| | 2111 | CD1 | LEU | 275 | 127.475 | 38.257 | 39.798 | 1.00 | 5.14 |
| | 2112 | CD2 | LEU | 275 | 127.812 | 38.960 | 42.179 | 1.00 | 9.22 |
| 20 | 2113 | C | LEU | 275 | 124.351 | 36.560 | 40.684 | 1.00 | 19.71 |
| | 2114 | O | LEU | 275 | 125.130 | 35.731 | 40.206 | 1.00 | 17.59 |
| | 2115 | N | GLY | 276 | 123.356 | 36.239 | 41.507 | 1.00 | 22.38 |
| | 2116 | CA | GLY | 276 | 123.098 | 34.860 | 41.880 | 1.00 | 15.02 |
| | 2117 | C | GLY | 276 | 122.429 | 34.101 | 40.747 | 1.00 | 8.27 |
| 25 | 2118 | O | GLY | 276 | 122.574 | 32.885 | 40.641 | 1.00 | 21.39 |
| | 2119 | N | VAL | 277 | 121.693 | 34.825 | 39.904 | 1.00 | 9.55 |
| | 2120 | CA | VAL | 277 | 120.992 | 34.245 | 38.758 | 1.00 | 6.19 |
| | 2121 | CB | VAL | 277 | 119.950 | 35.238 | 38.201 | 1.00 | 4.45 |
| | 2122 | CG1 | VAL | 277 | 119.236 | 34.660 | 36.994 | 1.00 | 2.00 |
| 30 | 2123 | CG2 | VAL | 277 | 118.946 | 35.576 | 39.284 | 1.00 | 2.00 |
| | 2124 | C | VAL | 277 | 122.003 | 33.848 | 37.686 | 1.00 | 9.32 |
| | 2125 | O | VAL | 277 | 121.872 | 32.807 | 37.042 | 1.00 | 17.27 |
| | 2126 | N | TYR | 278 | 122.992 | 34.711 | 37.481 | 1.00 | 13.83 |
| | 2127 | CA | TYR | 278 | 124.082 | 34.466 | 36.543 | 1.00 | 17.57 |
| 35 | 2128 | CB | TYR | 278 | 123.644 | 34.476 | 35.067 | 1.00 | 14.31 |
| | 2129 | CG | TYR | 278 | 122.485 | 35.368 | 34.675 | 1.00 | 21.92 |
| | 2130 | CD1 | TYR | 278 | 122.304 | 36.630 | 35.242 | 1.00 | 28.06 |
| | 2131 | CE1 | TYR | 278 | 121.249 | 37.454 | 34.839 | 1.00 | 17.69 |
| | 2132 | CD2 | TYR | 278 | 121.581 | 34.952 | 33.698 | 1.00 | 10.48 |
| 40 | 2133 | CE2 | TYR | 278 | 120.532 | 35.762 | 33.290 | 1.00 | 15.32 |
| | 2134 | CZ | TYR | 278 | 120.371 | 37.012 | 33.860 | 1.00 | 20.32 |
| | 2135 | OH | TYR | 278 | 119.341 | 37.820 | 33.432 | 1.00 | 16.49 |
| | 2136 | C | TYR | 278 | 125.236 | 35.423 | 36.790 | 1.00 | 22.42 |
| | 2137 | O | TYR | 278 | 125.024 | 36.609 | 37.052 | 1.00 | 24.68 |
| 45 | 2138 | N | PHE | 279 | 126.454 | 34.883 | 36.756 | 1.00 | 20.65 |
| | 2139 | CA | PHE | 279 | 127.665 | 35.662 | 36.998 | 1.00 | 24.23 |
| | 2140 | CB | PHE | 279 | 128.474 | 35.036 | 38.140 | 1.00 | 19.97 |
| | 2141 | CG | PHE | 279 | 129.063 | 33.694 | 37.800 | 1.00 | 27.50 |
| | 2142 | CD1 | PHE | 279 | 130.278 | 33.600 | 37.124 | 1.00 | 27.56 |
| 50 | 2143 | CD2 | PHE | 279 | 128.387 | 32.523 | 38.120 | 1.00 | 26.31 |

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|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 2144 | CE1 | PHE | 279 | 130.804 | 32.363 | 36.770 | 1.00 | 27.48 |
| | 2145 | CE2 | PHE | 279 | 128.906 | 31.283 | 37.770 | 1.00 | 27.51 |
| | 2146 | CZ | PHE | 279 | 130.116 | 31.202 | 37.093 | 1.00 | 26.58 |
| | 2147 | C | PHE | 279 | 128.564 | 35.797 | 35.773 | 1.00 | 22.60 |
| 5 | 2148 | O | PHE | 279 | 129.420 | 36.681 | 35.727 | 1.00 | 29.14 |
| | 2149 | N | GLU | 280 | 128.404 | 34.893 | 34.811 | 1.00 | 26.53 |
| | 2150 | CA | GLU | 280 | 129.217 | 34.909 | 33.599 | 1.00 | 25.23 |
| | 2151 | CB | GLU | 280 | 128.759 | 33.832 | 32.608 | 1.00 | 31.74 |
| | 2152 | CG | GLU | 280 | 129.004 | 32.392 | 33.056 | 1.00 | 26.55 |
| 10 | 2153 | CD | GLU | 280 | 127.873 | 31.806 | 33.899 | 1.00 | 40.41 |
| | 2154 | OE1 | GLU | 280 | 127.909 | 30.581 | 34.149 | 1.00 | 41.01 |
| | 2155 | OE2 | GLU | 280 | 126.949 | 32.549 | 34.307 | 1.00 | 31.27 |
| | 2156 | C | GLU | 280 | 129.195 | 36.276 | 32.928 | 1.00 | 28.72 |
| | 2157 | O | GLU | 280 | 128.169 | 36.958 | 32.918 | 1.00 | 21.31 |
| 15 | 2158 | N | PRO | 281 | 130.346 | 36.702 | 32.382 | 1.00 | 31.20 |
| | 2159 | CD | PRO | 281 | 131.607 | 35.942 | 32.368 | 1.00 | 29.80 |
| | 2160 | CA | PRO | 281 | 130.511 | 37.988 | 31.697 | 1.00 | 31.18 |
| | 2161 | CB | PRO | 281 | 131.976 | 37.949 | 31.246 | 1.00 | 36.16 |
| | 2162 | CG | PRO | 281 | 132.274 | 36.479 | 31.137 | 1.00 | 35.87 |
| 20 | 2163 | C | PRO | 281 | 129.561 | 38.213 | 30.522 | 1.00 | 29.70 |
| | 2164 | O | PRO | 281 | 129.196 | 39.352 | 30.226 | 1.00 | 29.95 |
| | 2165 | N | GLN | 282 | 129.161 | 37.126 | 29.866 | 1.00 | 27.63 |
| | 2166 | CA | GLN | 282 | 128.252 | 37.194 | 28.722 | 1.00 | 28.39 |
| | 2167 | CB | GLN | 282 | 128.174 | 35.832 | 28.028 | 1.00 | 34.10 |
| 25 | 2168 | CG | GLN | 282 | 127.630 | 34.717 | 28.912 | 1.00 | 45.80 |
| | 2169 | CD | GLN | 282 | 127.714 | 33.351 | 28.264 | 1.00 | 47.83 |
| | 2170 | OE1 | GLN | 282 | 128.543 | 32.523 | 28.647 | 1.00 | 54.06 |
| | 2171 | NE2 | GLN | 282 | 126.848 | 33.101 | 27.285 | 1.00 | 41.38 |
| | 2172 | C | GLN | 282 | 126.851 | 37.640 | 29.133 | 1.00 | 25.75 |
| 30 | 2173 | O | GLN | 282 | 126.061 | 38.071 | 28.294 | 1.00 | 34.41 |
| | 2174 | N | TYR | 283 | 126.553 | 37.521 | 30.425 | 1.00 | 26.54 |
| | 2175 | CA | TYR | 283 | 125.254 | 37.910 | 30.972 | 1.00 | 26.30 |
| | 2176 | CB | TYR | 283 | 124.765 | 36.853 | 31.966 | 1.00 | 19.61 |
| | 2177 | CG | TYR | 283 | 124.537 | 35.506 | 31.323 | 1.00 | 13.47 |
| 35 | 2178 | CD1 | TYR | 283 | 125.030 | 34.339 | 31.901 | 1.00 | 13.33 |
| | 2179 | CE1 | TYR | 283 | 124.852 | 33.099 | 31.286 | 1.00 | 15.49 |
| | 2180 | CD2 | TYR | 283 | 123.853 | 35.402 | 30.112 | 1.00 | 18.67 |
| | 2181 | CE2 | TYR | 283 | 123.669 | 34.173 | 29.490 | 1.00 | 23.42 |
| | 2182 | CZ | TYR | 283 | 124.172 | 33.026 | 30.079 | 1.00 | 14.24 |
| 40 | 2183 | OH | TYR | 283 | 124.002 | 31.817 | 29.448 | 1.00 | 22.41 |
| | 2184 | C | TYR | 283 | 125.304 | 39.287 | 31.632 | 1.00 | 29.24 |
| | 2185 | O | TYR | 283 | 124.504 | 39.599 | 32.517 | 1.00 | 27.80 |
| | 2186 | N | SER | 284 | 126.244 | 40.108 | 31.170 | 1.00 | 29.09 |
| | 2187 | CA | SER | 284 | 126.438 | 41.461 | 31.673 | 1.00 | 24.35 |
| 45 | 2188 | CB | SER | 284 | 127.644 | 42.103 | 30.981 | 1.00 | 29.60 |
| | 2189 | OG | SER | 284 | 127.873 | 43.418 | 31.456 | 1.00 | 29.67 |
| | 2190 | C | SER | 284 | 125.192 | 42.315 | 31.451 | 1.00 | 23.95 |
| | 2191 | O | SER | 284 | 124.647 | 42.882 | 32.396 | 1.00 | 16.24 |
| | 2192 | N | GLN | 285 | 124.743 | 42.393 | 30.199 | 1.00 | 29.77 |
| 50 | 2193 | CA | GLN | 285 | 123.556 | 43.173 | 29.852 | 1.00 | 36.37 |

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|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 2194 | CB | GLN | 285 | 123.313 | 43.138 | 28.339 | 1.00 | 36.36 |
| | 2195 | CG | GLN | 285 | 122.119 | 43.974 | 27.883 | 1.00 | 42.33 |
| | 2196 | CD | GLN | 285 | 121.887 | 43.913 | 26.382 | 1.00 | 47.38 |
| 5 | 2197 | OE1 | GLN | 285 | 122.208 | 42.919 | 25.727 | 1.00 | 45.82 |
| | 2198 | NE2 | GLN | 285 | 121.321 | 44.981 | 25.832 | 1.00 | 47.01 |
| | 2199 | C | GLN | 285 | 122.328 | 42.638 | 30.588 | 1.00 | 40.35 |
| | 2200 | O | GLN | 285 | 121.503 | 43.413 | 31.076 | 1.00 | 46.67 |
| | 2201 | N | ALA | 286 | 122.242 | 41.312 | 30.686 | 1.00 | 38.34 |
| 10 | 2202 | CA | ALA | 286 | 121.136 | 40.637 | 31.356 | 1.00 | 27.14 |
| | 2203 | CB | ALA | 286 | 121.252 | 39.136 | 31.170 | 1.00 | 34.43 |
| | 2204 | C | ALA | 286 | 121.067 | 40.983 | 32.837 | 1.00 | 24.71 |
| | 2205 | O | ALA | 286 | 119.996 | 41.319 | 33.346 | 1.00 | 32.18 |
| | 2206 | N | ARG | 287 | 122.203 | 40.891 | 33.526 | 1.00 | 17.67 |
| 15 | 2207 | CA | ARG | 287 | 122.261 | 41.212 | 34.951 | 1.00 | 17.77 |
| | 2208 | CB | ARG | 287 | 123.680 | 41.046 | 35.504 | 1.00 | 14.04 |
| | 2209 | CG | ARG | 287 | 124.013 | 39.659 | 36.008 | 1.00 | 21.57 |
| | 2210 | CD | ARG | 287 | 125.294 | 39.673 | 36.828 | 1.00 | 20.38 |
| | 2211 | NE | ARG | 287 | 126.451 | 40.078 | 36.033 | 1.00 | 14.48 |
| | 2212 | CZ | ARG | 287 | 127.080 | 39.293 | 35.162 | 1.00 | 22.09 |
| 20 | 2213 | NH1 | ARG | 287 | 126.670 | 38.049 | 34.959 | 1.00 | 17.96 |
| | 2214 | NH2 | ARG | 287 | 128.132 | 39.749 | 34.497 | 1.00 | 25.61 |
| | 2215 | C | ARG | 287 | 121.802 | 42.642 | 35.207 | 1.00 | 24.30 |
| | 2216 | O | ARG | 287 | 120.942 | 42.877 | 36.046 | 1.00 | 22.53 |
| 25 | 2217 | N | VAL | 288 | 122.358 | 43.583 | 34.449 | 1.00 | 32.79 |
| | 2218 | CA | VAL | 288 | 122.031 | 45.001 | 34.586 | 1.00 | 35.93 |
| | 2219 | CB | VAL | 288 | 122.800 | 45.853 | 33.543 | 1.00 | 42.80 |
| | 2220 | CG1 | VAL | 288 | 122.484 | 47.329 | 33.718 | 1.00 | 45.42 |
| | 2221 | CG2 | VAL | 288 | 124.294 | 45.622 | 33.682 | 1.00 | 39.26 |
| | 2222 | C | VAL | 288 | 120.525 | 45.246 | 34.470 | 1.00 | 30.79 |
| 30 | 2223 | O | VAL | 288 | 119.927 | 45.888 | 35.339 | 1.00 | 27.62 |
| | 2224 | N | MET | 289 | 119.914 | 44.698 | 33.422 | 1.00 | 25.59 |
| | 2225 | CA | MET | 289 | 118.473 | 44.837 | 33.202 | 1.00 | 20.40 |
| | 2226 | CB | MET | 289 | 118.055 | 44.123 | 31.908 | 1.00 | 11.02 |
| | 2227 | CG | MET | 289 | 118.675 | 44.684 | 30.646 | 1.00 | 17.69 |
| 35 | 2228 | SD | MET | 289 | 118.236 | 43.769 | 29.151 | 1.00 | 29.61 |
| | 2229 | CE | MET | 289 | 117.076 | 44.873 | 28.424 | 1.00 | 23.00 |
| | 2230 | C | MET | 289 | 117.692 | 44.246 | 34.383 | 1.00 | 20.89 |
| | 2231 | O | MET | 289 | 116.762 | 44.861 | 34.901 | 1.00 | 25.06 |
| | 2232 | N | LEU | 290 | 118.104 | 43.063 | 34.825 | 1.00 | 20.72 |
| 40 | 2233 | CA | LEU | 290 | 117.448 | 42.379 | 35.935 | 1.00 | 15.74 |
| | 2234 | CB | LEU | 290 | 118.020 | 40.969 | 36.078 | 1.00 | 14.98 |
| | 2235 | CG | LEU | 290 | 117.497 | 40.044 | 37.174 | 1.00 | 16.12 |
| | 2236 | CD1 | LEU | 290 | 115.981 | 39.981 | 37.142 | 1.00 | 16.37 |
| | 2237 | CD2 | LEU | 290 | 118.098 | 38.659 | 36.964 | 1.00 | 19.76 |
| 45 | 2238 | C | LEU | 290 | 117.530 | 43.139 | 37.261 | 1.00 | 21.50 |
| | 2239 | O | LEU | 290 | 116.561 | 43.172 | 38.019 | 1.00 | 23.53 |
| | 2240 | N | VAL | 291 | 118.675 | 43.761 | 37.534 | 1.00 | 24.67 |
| | 2241 | CA | VAL | 291 | 118.858 | 44.518 | 38.773 | 1.00 | 28.92 |
| | 2242 | CB | VAL | 291 | 120.280 | 45.113 | 38.893 | 1.00 | 30.77 |
| 50 | 2243 | CG1 | VAL | 291 | 120.439 | 45.822 | 40.234 | 1.00 | 27.10 |

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|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 2244 | CG2 | VAL | 291 | 121.324 | 44.033 | 38.742 | 1.00 | 35.91 |
| | 2245 | C | VAL | 291 | 117.872 | 45.679 | 38.826 | 1.00 | 33.69 |
| | 2246 | O | VAL | 291 | 117.266 | 45.950 | 39.867 | 1.00 | 38.64 |
| | 2247 | N | LYS | 292 | 117.722 | 46.360 | 37.693 | 1.00 | 32.65 |
| 5 | 2248 | CA | LYS | 292 | 116.819 | 47.500 | 37.589 | 1.00 | 29.16 |
| | 2249 | CB | LYS | 292 | 116.961 | 48.155 | 36.213 | 1.00 | 28.67 |
| | 2250 | CG | LYS | 292 | 118.314 | 48.814 | 35.986 | 1.00 | 28.14 |
| | 2251 | CD | LYS | 292 | 118.440 | 49.353 | 34.575 | 1.00 | 36.09 |
| | 2252 | CE | LYS | 292 | 119.765 | 50.059 | 34.370 | 1.00 | 37.49 |
| 10 | 2253 | NZ | LYS | 292 | 119.962 | 50.417 | 32.940 | 1.00 | 42.24 |
| | 2254 | C | LYS | 292 | 115.369 | 47.102 | 37.849 | 1.00 | 25.46 |
| | 2255 | O | LYS | 292 | 114.633 | 47.829 | 38.514 | 1.00 | 23.99 |
| | 2256 | N | THR | 293 | 114.984 | 45.922 | 37.365 | 1.00 | 28.08 |
| | 2257 | CA | THR | 293 | 113.627 | 45.401 | 37.536 | 1.00 | 20.11 |
| 15 | 2258 | CB | THR | 293 | 113.385 | 44.183 | 36.617 | 1.00 | 19.93 |
| | 2259 | OG1 | THR | 293 | 113.325 | 44.619 | 35.252 | 1.00 | 19.22 |
| | 2260 | CG2 | THR | 293 | 112.095 | 43.472 | 36.972 | 1.00 | 14.44 |
| | 2261 | C | THR | 293 | 113.326 | 45.026 | 38.987 | 1.00 | 22.63 |
| | 2262 | O | THR | 293 | 112.286 | 45.405 | 39.524 | 1.00 | 30.10 |
| 20 | 2263 | N | ILE | 294 | 114.239 | 44.295 | 39.621 | 1.00 | 23.15 |
| | 2264 | CA | ILE | 294 | 114.058 | 43.884 | 41.015 | 1.00 | 22.01 |
| | 2265 | CB | ILE | 294 | 115.232 | 43.007 | 41.522 | 1.00 | 19.34 |
| | 2266 | CG2 | ILE | 294 | 114.962 | 42.546 | 42.958 | 1.00 | 19.45 |
| | 2267 | CG1 | ILE | 294 | 115.430 | 41.799 | 40.604 | 1.00 | 12.44 |
| 25 | 2268 | CD1 | ILE | 294 | 116.564 | 40.876 | 41.017 | 1.00 | 23.70 |
| | 2269 | C | ILE | 294 | 113.959 | 45.113 | 41.910 | 1.00 | 21.14 |
| | 2270 | O | ILE | 294 | 113.097 | 45.193 | 42.789 | 1.00 | 23.19 |
| | 2271 | N | SER | 295 | 114.841 | 46.075 | 41.664 | 1.00 | 27.23 |
| | 2272 | CA | SER | 295 | 114.879 | 47.310 | 42.435 | 1.00 | 36.44 |
| 30 | 2273 | CB | SER | 295 | 116.063 | 48.167 | 41.979 | 1.00 | 38.02 |
| | 2274 | OG | SER | 295 | 116.508 | 49.015 | 43.021 | 1.00 | 50.33 |
| | 2275 | C | SER | 295 | 113.566 | 48.077 | 42.265 | 1.00 | 33.20 |
| | 2276 | O | SER | 295 | 112.984 | 48.562 | 43.239 | 1.00 | 27.63 |
| | 2277 | N | MET | 296 | 113.083 | 48.124 | 41.026 | 1.00 | 32.18 |
| 35 | 2278 | CA | MET | 296 | 111.843 | 48.816 | 40.685 | 1.00 | 33.20 |
| | 2279 | CB | MET | 296 | 111.659 | 48.829 | 39.165 | 1.00 | 33.02 |
| | 2280 | CG | MET | 296 | 110.820 | 49.978 | 38.637 | 1.00 | 34.84 |
| | 2281 | SD | MET | 296 | 111.653 | 51.571 | 38.807 | 1.00 | 40.22 |
| | 2282 | CE | MET | 296 | 110.937 | 52.162 | 40.336 | 1.00 | 31.58 |
| 40 | 2283 | C | MET | 296 | 110.617 | 48.181 | 41.343 | 1.00 | 36.25 |
| | 2284 | O | MET | 296 | 109.831 | 48.871 | 41.997 | 1.00 | 35.27 |
| | 2285 | N | ILE | 297 | 110.462 | 46.867 | 41.172 | 1.00 | 36.41 |
| | 2286 | CA | ILE | 297 | 109.327 | 46.145 | 41.743 | 1.00 | 31.22 |
| | 2287 | CB | ILE | 297 | 109.240 | 44.681 | 41.222 | 1.00 | 30.61 |
| 45 | 2288 | CG2 | ILE | 297 | 110.401 | 43.850 | 41.748 | 1.00 | 32.13 |
| | 2289 | CG1 | ILE | 297 | 107.915 | 44.039 | 41.647 | 1.00 | 25.21 |
| | 2290 | CD1 | ILE | 297 | 106.681 | 44.725 | 41.088 | 1.00 | 9.77 |
| | 2291 | C | ILE | 297 | 109.362 | 46.151 | 43.266 | 1.00 | 28.01 |
| | 2292 | O | ILE | 297 | 108.333 | 45.964 | 43.914 | 1.00 | 33.37 |
| 50 | 2293 | N | SER | 298 | 110.544 | 46.369 | 43.834 | 1.00 | 26.49 |

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|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 2294 | CA | SER | 298 | 110.682 | 46.410 | 45.284 | 1.00 | 31.31 |
| | 2295 | CB | SER | 298 | 112.152 | 46.511 | 45.692 | 1.00 | 36.65 |
| | 2296 | OG | SER | 298 | 112.281 | 46.533 | 47.106 | 1.00 | 34.52 |
| | 2297 | C | SER | 298 | 109.921 | 47.616 | 45.810 | 1.00 | 31.13 |
| 5 | 2298 | O | SER | 298 | 109.331 | 47.567 | 46.888 | 1.00 | 32.44 |
| | 2299 | N | ILE | 299 | 109.932 | 48.693 | 45.029 | 1.00 | 31.80 |
| | 2300 | CA | ILE | 299 | 109.239 | 49.923 | 45.390 | 1.00 | 37.55 |
| | 2301 | CB | ILE | 299 | 109.648 | 51.086 | 44.462 | 1.00 | 44.76 |
| | 2302 | CG2 | ILE | 299 | 108.809 | 52.326 | 44.753 | 1.00 | 45.64 |
| 10 | 2303 | CG1 | ILE | 299 | 111.135 | 51.390 | 44.645 | 1.00 | 46.63 |
| | 2304 | CD1 | ILE | 299 | 111.656 | 52.438 | 43.707 | 1.00 | 51.58 |
| | 2305 | C | ILE | 299 | 107.735 | 49.710 | 45.315 | 1.00 | 31.48 |
| | 2306 | O | ILE | 299 | 107.008 | 50.072 | 46.238 | 1.00 | 32.42 |
| | 2307 | N | VAL | 300 | 107.277 | 49.101 | 44.224 | 1.00 | 27.09 |
| 15 | 2308 | CA | VAL | 300 | 105.855 | 48.824 | 44.037 | 1.00 | 23.95 |
| | 2309 | CB | VAL | 300 | 105.598 | 48.080 | 42.709 | 1.00 | 22.51 |
| | 2310 | CG1 | VAL | 300 | 104.108 | 47.876 | 42.494 | 1.00 | 20.37 |
| | 2311 | CG2 | VAL | 300 | 106.190 | 48.867 | 41.552 | 1.00 | 20.21 |
| | 2312 | C | VAL | 300 | 105.349 | 47.990 | 45.211 | 1.00 | 23.59 |
| 20 | 2313 | O | VAL | 300 | 104.247 | 48.204 | 45.714 | 1.00 | 30.31 |
| | 2314 | N | ASP | 301 | 106.186 | 47.072 | 45.674 | 1.00 | 24.66 |
| | 2315 | CA | ASP | 301 | 105.837 | 46.226 | 46.802 | 1.00 | 31.65 |
| | 2316 | CB | ASP | 301 | 106.879 | 45.121 | 46.975 | 1.00 | 25.48 |
| | 2317 | CG | ASP | 301 | 106.523 | 44.163 | 48.087 | 1.00 | 24.95 |
| 25 | 2318 | OD1 | ASP | 301 | 105.672 | 43.277 | 47.869 | 1.00 | 37.24 |
| | 2319 | OD2 | ASP | 301 | 107.075 | 44.309 | 49.193 | 1.00 | 32.62 |
| | 2320 | C | ASP | 301 | 105.762 | 47.078 | 48.065 | 1.00 | 33.30 |
| | 2321 | O | ASP | 301 | 104.847 | 46.930 | 48.874 | 1.00 | 36.41 |
| | 2322 | N | ASP | 302 | 106.737 | 47.971 | 48.218 | 1.00 | 41.65 |
| 30 | 2323 | CA | ASP | 302 | 106.805 | 48.866 | 49.369 | 1.00 | 43.94 |
| | 2324 | CB | ASP | 302 | 108.124 | 49.650 | 49.353 | 1.00 | 49.38 |
| | 2325 | CG | ASP | 302 | 109.322 | 48.798 | 49.744 | 1.00 | 55.74 |
| | 2326 | OD1 | ASP | 302 | 109.246 | 48.101 | 50.780 | 1.00 | 59.49 |
| | 2327 | OD2 | ASP | 302 | 110.344 | 48.833 | 49.024 | 1.00 | 52.10 |
| 35 | 2328 | C | ASP | 302 | 105.619 | 49.831 | 49.416 | 1.00 | 43.11 |
| | 2329 | O | ASP | 302 | 105.198 | 50.257 | 50.493 | 1.00 | 44.18 |
| | 2330 | N | THR | 303 | 105.081 | 50.159 | 48.243 | 1.00 | 38.88 |
| | 2331 | CA | THR | 303 | 103.945 | 51.069 | 48.123 | 1.00 | 33.20 |
| | 2332 | CB | THR | 303 | 103.745 | 51.514 | 46.660 | 1.00 | 41.14 |
| 40 | 2333 | OG1 | THR | 303 | 104.965 | 52.075 | 46.158 | 1.00 | 39.42 |
| | 2334 | CG2 | THR | 303 | 102.643 | 52.555 | 46.564 | 1.00 | 44.39 |
| | 2335 | C | THR | 303 | 102.652 | 50.426 | 48.624 | 1.00 | 36.28 |
| | 2336 | O | THR | 303 | 101.930 | 51.016 | 49.425 | 1.00 | 44.91 |
| | 2337 | N | PHE | 304 | 102.367 | 49.218 | 48.143 | 1.00 | 33.21 |
| 45 | 2338 | CA | PHE | 304 | 101.167 | 48.478 | 48.532 | 1.00 | 26.28 |
| | 2339 | CB | PHE | 304 | 101.005 | 47.234 | 47.653 | 1.00 | 23.04 |
| | 2340 | CG | PHE | 304 | 100.431 | 47.509 | 46.293 | 1.00 | 14.95 |
| | 2341 | CD1 | PHE | 304 | 101.250 | 47.901 | 45.239 | 1.00 | 16.64 |
| | 2342 | CD2 | PHE | 304 | 99.068 | 47.352 | 46.059 | 1.00 | 16.64 |
| 50 | 2343 | CE1 | PHE | 304 | 100.720 | 48.132 | 43.968 | 1.00 | 20.58 |

| | | | | | | | | | |
|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 2344 | CE2 | PHE | 304 | 98.527 | 47.580 | 44.793 | 1.00 | 13.24 |
| | 2345 | CZ | PHE | 304 | 99.355 | 47.971 | 43.746 | 1.00 | 15.28 |
| | 2346 | C | PHE | 304 | 101.183 | 48.032 | 49.993 | 1.00 | 34.53 |
| | 2347 | O | PHE | 304 | 100.135 | 47.926 | 50.632 | 1.00 | 38.46 |
| 5 | 2348 | N | ASP | 305 | 102.379 | 47.778 | 50.515 | 1.00 | 40.19 |
| | 2349 | CA | ASP | 305 | 102.544 | 47.300 | 51.881 | 1.00 | 46.42 |
| | 2350 | CB | ASP | 305 | 103.774 | 46.399 | 51.968 | 1.00 | 58.96 |
| | 2351 | CG | ASP | 305 | 103.431 | 44.933 | 51.845 | 1.00 | 70.39 |
| | 2352 | OD1 | ASP | 305 | 102.647 | 44.572 | 50.940 | 1.00 | 75.74 |
| 10 | 2353 | OD2 | ASP | 305 | 103.957 | 44.140 | 52.656 | 1.00 | 75.60 |
| | 2354 | C | ASP | 305 | 102.605 | 48.324 | 53.001 | 1.00 | 47.79 |
| | 2355 | O | ASP | 305 | 101.936 | 48.161 | 54.022 | 1.00 | 46.25 |
| | 2356 | N | ALA | 306 | 103.425 | 49.357 | 52.831 | 1.00 | 52.07 |
| | 2357 | CA | ALA | 306 | 103.574 | 50.362 | 53.875 | 1.00 | 54.53 |
| 15 | 2358 | CB | ALA | 306 | 104.958 | 50.240 | 54.518 | 1.00 | 57.28 |
| | 2359 | C | ALA | 306 | 103.312 | 51.807 | 53.462 | 1.00 | 53.39 |
| | 2360 | O | ALA | 306 | 103.971 | 52.718 | 53.965 | 1.00 | 58.62 |
| | 2361 | N | TYR | 307 | 102.345 | 52.030 | 52.576 | 1.00 | 51.30 |
| | 2362 | CA | TYR | 307 | 102.045 | 53.395 | 52.165 | 1.00 | 53.81 |
| 20 | 2363 | CB | TYR | 307 | 103.107 | 53.918 | 51.195 | 1.00 | 48.52 |
| | 2364 | CG | TYR | 307 | 103.396 | 55.388 | 51.392 | 1.00 | 55.69 |
| | 2365 | CD1 | TYR | 307 | 103.963 | 55.847 | 52.581 | 1.00 | 59.86 |
| | 2366 | CE1 | TYR | 307 | 104.206 | 57.200 | 52.789 | 1.00 | 62.54 |
| | 2367 | CD2 | TYR | 307 | 103.077 | 56.324 | 50.411 | 1.00 | 56.20 |
| 25 | 2368 | CE2 | TYR | 307 | 103.315 | 57.683 | 50.608 | 1.00 | 59.89 |
| | 2369 | CZ | TYR | 307 | 103.878 | 58.112 | 51.801 | 1.00 | 62.92 |
| | 2370 | OH | TYR | 307 | 104.112 | 59.451 | 52.009 | 1.00 | 66.19 |
| | 2371 | C | TYR | 307 | 100.647 | 53.640 | 51.597 | 1.00 | 59.33 |
| | 2372 | O | TYR | 307 | 99.752 | 54.078 | 52.320 | 1.00 | 66.09 |
| 30 | 2373 | N | GLY | 308 | 100.473 | 53.364 | 50.307 | 1.00 | 59.69 |
| | 2374 | CA | GLY | 308 | 99.199 | 53.580 | 49.636 | 1.00 | 58.39 |
| | 2375 | C | GLY | 308 | 97.924 | 53.122 | 50.326 | 1.00 | 60.86 |
| | 2376 | O | GLY | 308 | 97.925 | 52.163 | 51.101 | 1.00 | 61.04 |
| | 2377 | N | THR | 309 | 96.833 | 53.833 | 50.044 | 1.00 | 60.72 |
| 35 | 2378 | CA | THR | 309 | 95.522 | 53.524 | 50.609 | 1.00 | 57.07 |
| | 2379 | CB | THR | 309 | 94.751 | 54.807 | 50.989 | 1.00 | 55.19 |
| | 2380 | OG1 | THR | 309 | 94.651 | 55.667 | 49.847 | 1.00 | 47.62 |
| | 2381 | CG2 | THR | 309 | 95.461 | 55.538 | 52.117 | 1.00 | 46.57 |
| | 2382 | C | THR | 309 | 94.693 | 52.722 | 49.609 | 1.00 | 59.08 |
| 40 | 2383 | O | THR | 309 | 94.996 | 52.709 | 48.415 | 1.00 | 56.21 |
| | 2384 | N | VAL | 310 | 93.631 | 52.089 | 50.107 | 1.00 | 60.80 |
| | 2385 | CA | VAL | 310 | 92.737 | 51.264 | 49.295 | 1.00 | 62.84 |
| | 2386 | CB | VAL | 310 | 91.430 | 50.932 | 50.059 | 1.00 | 64.23 |
| | 2387 | CG1 | VAL | 310 | 90.667 | 49.821 | 49.351 | 1.00 | 66.80 |
| 45 | 2388 | CG2 | VAL | 310 | 91.737 | 50.534 | 51.498 | 1.00 | 61.87 |
| | 2389 | C | VAL | 310 | 92.390 | 51.903 | 47.947 | 1.00 | 63.74 |
| | 2390 | O | VAL | 310 | 92.469 | 51.244 | 46.904 | 1.00 | 60.65 |
| | 2391 | N | LYS | 311 | 92.038 | 53.189 | 47.972 | 1.00 | 65.40 |
| | 2392 | CA | LYS | 311 | 91.687 | 53.926 | 46.755 | 1.00 | 65.81 |
| 50 | 2393 | CB | LYS | 311 | 91.121 | 55.301 | 47.105 | 1.00 | 70.45 |

| | | | | | | | | | |
|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 2394 | CG | LYS | 311 | 89.696 | 55.305 | 47.621 | 1.00 | 74.65 |
| | 2395 | CD | LYS | 311 | 89.175 | 56.734 | 47.692 | 1.00 | 77.16 |
| | 2396 | CE | LYS | 311 | 87.719 | 56.787 | 48.120 | 1.00 | 75.45 |
| | 2397 | NZ | LYS | 311 | 87.239 | 58.194 | 48.137 | 1.00 | 78.70 |
| 5 | 2398 | C | LYS | 311 | 92.889 | 54.116 | 45.842 | 1.00 | 63.97 |
| | 2399 | O | LYS | 311 | 92.840 | 53.788 | 44.658 | 1.00 | 64.41 |
| | 2400 | N | GLU | 312 | 93.961 | 54.670 | 46.403 | 1.00 | 60.54 |
| | 2401 | CA | GLU | 312 | 95.195 | 54.931 | 45.665 | 1.00 | 57.43 |
| | 2402 | CB | GLU | 312 | 96.263 | 55.516 | 46.596 | 1.00 | 59.85 |
| 10 | 2403 | CG | GLU | 312 | 95.900 | 56.859 | 47.194 | 1.00 | 66.27 |
| | 2404 | CD | GLU | 312 | 97.024 | 57.438 | 48.033 | 1.00 | 69.45 |
| | 2405 | OE1 | GLU | 312 | 97.396 | 56.817 | 49.051 | 1.00 | 71.29 |
| | 2406 | OE2 | GLU | 312 | 97.544 | 58.514 | 47.666 | 1.00 | 70.23 |
| | 2407 | C | GLU | 312 | 95.750 | 53.679 | 44.989 | 1.00 | 53.28 |
| 15 | 2408 | O | GLU | 312 | 96.133 | 53.715 | 43.815 | 1.00 | 44.50 |
| | 2409 | N | LEU | 313 | 95.787 | 52.577 | 45.736 | 1.00 | 45.10 |
| | 2410 | CA | LEU | 313 | 96.290 | 51.310 | 45.222 | 1.00 | 40.42 |
| | 2411 | CB | LEU | 313 | 96.361 | 50.267 | 46.343 | 1.00 | 35.64 |
| | 2412 | CG | LEU | 313 | 97.263 | 50.614 | 47.534 | 1.00 | 32.14 |
| 20 | 2413 | CD1 | LEU | 313 | 97.226 | 49.501 | 48.569 | 1.00 | 28.15 |
| | 2414 | CD2 | LEU | 313 | 98.687 | 50.861 | 47.061 | 1.00 | 26.11 |
| | 2415 | C | LEU | 313 | 95.430 | 50.800 | 44.071 | 1.00 | 41.37 |
| | 2416 | O | LEU | 313 | 95.950 | 50.275 | 43.085 | 1.00 | 39.82 |
| | 2417 | N | GLU | 314 | 94.116 | 50.981 | 44.193 | 1.00 | 41.16 |
| 25 | 2418 | CA | GLU | 314 | 93.180 | 50.553 | 43.156 | 1.00 | 41.35 |
| | 2419 | CB | GLU | 314 | 91.737 | 50.728 | 43.636 | 1.00 | 45.36 |
| | 2420 | CG | GLU | 314 | 90.674 | 50.326 | 42.612 | 1.00 | 51.16 |
| | 2421 | CD | GLU | 314 | 90.717 | 48.848 | 42.251 | 1.00 | 56.61 |
| | 2422 | OE1 | GLU | 314 | 90.469 | 48.007 | 43.144 | 1.00 | 55.46 |
| 30 | 2423 | OE2 | GLU | 314 | 90.988 | 48.530 | 41.071 | 1.00 | 49.16 |
| | 2424 | C | GLU | 314 | 93.417 | 51.357 | 41.880 | 1.00 | 38.64 |
| | 2425 | O | GLU | 314 | 93.315 | 50.828 | 40.772 | 1.00 | 41.77 |
| | 2426 | N | ALA | 315 | 93.742 | 52.634 | 42.047 | 1.00 | 37.56 |
| | 2427 | CA | ALA | 315 | 94.012 | 53.513 | 40.917 | 1.00 | 37.09 |
| 35 | 2428 | CB | ALA | 315 | 94.024 | 54.961 | 41.375 | 1.00 | 41.02 |
| | 2429 | C | ALA | 315 | 95.354 | 53.146 | 40.292 | 1.00 | 37.51 |
| | 2430 | O | ALA | 315 | 95.522 | 53.222 | 39.074 | 1.00 | 40.72 |
| | 2431 | N | TYR | 316 | 96.301 | 52.741 | 41.138 | 1.00 | 37.47 |
| | 2432 | CA | TYR | 316 | 97.641 | 52.351 | 40.698 | 1.00 | 36.60 |
| 40 | 2433 | CB | TYR | 316 | 98.567 | 52.189 | 41.908 | 1.00 | 42.76 |
| | 2434 | CG | TYR | 316 | 100.045 | 52.214 | 41.576 | 1.00 | 47.70 |
| | 2435 | CD1 | TYR | 316 | 100.701 | 53.421 | 41.323 | 1.00 | 50.35 |
| | 2436 | CE1 | TYR | 316 | 102.064 | 53.456 | 41.029 | 1.00 | 47.09 |
| | 2437 | CD2 | TYR | 316 | 100.792 | 51.038 | 41.526 | 1.00 | 50.58 |
| 45 | 2438 | CE2 | TYR | 316 | 102.158 | 51.063 | 41.232 | 1.00 | 51.96 |
| | 2439 | CZ | TYR | 316 | 102.785 | 52.276 | 40.986 | 1.00 | 46.31 |
| | 2440 | OH | TYR | 316 | 104.130 | 52.308 | 40.697 | 1.00 | 45.69 |
| | 2441 | C | TYR | 316 | 97.582 | 51.047 | 39.909 | 1.00 | 38.30 |
| | 2442 | O | TYR | 316 | 98.142 | 50.949 | 38.812 | 1.00 | 29.96 |
| 50 | 2443 | N | THR | 317 | 96.890 | 50.058 | 40.473 | 1.00 | 34.49 |

| | | | | | | | | | |
|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 2444 | CA | THR | 317 | 96.731 | 48.752 | 39.839 | 1.00 | 33.58 |
| | 2445 | CB | THR | 317 | 95.811 | 47.831 | 40.671 | 1.00 | 29.35 |
| | 2446 | OG1 | THR | 317 | 96.347 | 47.676 | 41.990 | 1.00 | 30.19 |
| 5 | 2447 | CG2 | THR | 317 | 95.691 | 46.460 | 40.020 | 1.00 | 28.64 |
| | 2448 | C | THR | 317 | 96.125 | 48.922 | 38.448 | 1.00 | 38.84 |
| | 2449 | O | THR | 317 | 96.624 | 48.363 | 37.470 | 1.00 | 37.70 |
| | 2450 | N | ASP | 318 | 95.070 | 49.731 | 38.369 | 1.00 | 39.63 |
| | 2451 | CA | ASP | 318 | 94.385 | 49.987 | 37.110 | 1.00 | 43.25 |
| 10 | 2452 | CB | ASP | 318 | 93.115 | 50.806 | 37.351 | 1.00 | 53.81 |
| | 2453 | CG | ASP | 318 | 92.282 | 50.972 | 36.094 | 1.00 | 64.26 |
| | 2454 | OD1 | ASP | 318 | 91.830 | 49.947 | 35.538 | 1.00 | 68.93 |
| | 2455 | OD2 | ASP | 318 | 92.088 | 52.126 | 35.656 | 1.00 | 69.91 |
| | 2456 | C | ASP | 318 | 95.292 | 50.706 | 36.118 | 1.00 | 38.89 |
| | 2457 | O | ASP | 318 | 95.280 | 50.406 | 34.922 | 1.00 | 35.65 |
| 15 | 2458 | N | ALA | 319 | 96.081 | 51.651 | 36.622 | 1.00 | 39.85 |
| | 2459 | CA | ALA | 319 | 97.001 | 52.409 | 35.783 | 1.00 | 39.48 |
| | 2460 | CB | ALA | 319 | 97.716 | 53.462 | 36.610 | 1.00 | 45.21 |
| | 2461 | C | ALA | 319 | 98.007 | 51.469 | 35.123 | 1.00 | 36.47 |
| 20 | 2462 | O | ALA | 319 | 98.261 | 51.564 | 33.920 | 1.00 | 28.06 |
| | 2463 | N | ILE | 320 | 98.547 | 50.541 | 35.912 | 1.00 | 36.88 |
| | 2464 | CA | ILE | 320 | 99.514 | 49.560 | 35.422 | 1.00 | 35.98 |
| | 2465 | CB | ILE | 320 | 99.994 | 48.620 | 36.561 | 1.00 | 43.40 |
| | 2466 | CG2 | ILE | 320 | 100.784 | 47.443 | 35.991 | 1.00 | 44.99 |
| | 2467 | CG1 | ILE | 320 | 100.834 | 49.397 | 37.582 | 1.00 | 45.58 |
| 25 | 2468 | CD1 | ILE | 320 | 102.173 | 49.891 | 37.054 | 1.00 | 39.26 |
| | 2469 | C | ILE | 320 | 98.911 | 48.712 | 34.307 | 1.00 | 31.85 |
| | 2470 | O | ILE | 320 | 99.544 | 48.506 | 33.271 | 1.00 | 32.45 |
| | 2471 | N | GLN | 321 | 97.680 | 48.245 | 34.518 | 1.00 | 27.13 |
| 30 | 2472 | CA | GLN | 321 | 96.980 | 47.414 | 33.538 | 1.00 | 29.80 |
| | 2473 | CB | GLN | 321 | 95.592 | 47.021 | 34.053 | 1.00 | 37.41 |
| | 2474 | CG | GLN | 321 | 95.581 | 46.336 | 35.422 | 1.00 | 37.33 |
| | 2475 | CD | GLN | 321 | 96.510 | 45.136 | 35.508 | 1.00 | 42.33 |
| | 2476 | OE1 | GLN | 321 | 96.690 | 44.398 | 34.536 | 1.00 | 43.16 |
| | 2477 | NE2 | GLN | 321 | 97.108 | 44.938 | 36.679 | 1.00 | 35.06 |
| 35 | 2478 | C | GLN | 321 | 96.856 | 48.101 | 32.180 | 1.00 | 30.46 |
| | 2479 | O | GLN | 321 | 97.066 | 47.474 | 31.139 | 1.00 | 25.13 |
| | 2480 | N | ARG | 322 | 96.519 | 49.390 | 32.199 | 1.00 | 36.61 |
| | 2481 | CA | ARG | 322 | 96.384 | 50.171 | 30.971 | 1.00 | 40.97 |
| 40 | 2482 | CB | ARG | 322 | 95.779 | 51.549 | 31.264 | 1.00 | 48.13 |
| | 2483 | CG | ARG | 322 | 94.261 | 51.612 | 31.176 | 1.00 | 58.29 |
| | 2484 | CD | ARG | 322 | 93.581 | 50.836 | 32.290 | 1.00 | 66.64 |
| | 2485 | NE | ARG | 322 | 92.125 | 50.822 | 32.134 | 1.00 | 76.38 |
| | 2486 | CZ | ARG | 322 | 91.326 | 51.868 | 32.344 | 1.00 | 74.78 |
| | 2487 | NH1 | ARG | 322 | 91.827 | 53.035 | 32.727 | 1.00 | 73.98 |
| 45 | 2488 | NH2 | ARG | 322 | 90.019 | 51.751 | 32.157 | 1.00 | 73.84 |
| | 2489 | C | ARG | 322 | 97.737 | 50.347 | 30.290 | 1.00 | 39.65 |
| | 2490 | O | ARG | 322 | 97.848 | 50.233 | 29.067 | 1.00 | 46.16 |
| | 2491 | N | TRP | 323 | 98.757 | 50.635 | 31.094 | 1.00 | 37.39 |
| | 2492 | CA | TRP | 323 | 100.118 | 50.828 | 30.607 | 1.00 | 35.58 |
| 50 | 2493 | CB | TRP | 323 | 100.663 | 49.535 | 29.990 | 1.00 | 36.83 |

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|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 2494 | CG | TRP | 323 | 102.169 | 49.447 | 29.979 | 1.00 | 41.47 |
| | 2495 | CD2 | TRP | 323 | 103.017 | 49.048 | 31.063 | 1.00 | 38.37 |
| | 2496 | CE2 | TRP | 323 | 104.351 | 49.089 | 30.594 | 1.00 | 38.29 |
| 5 | 2497 | CE3 | TRP | 323 | 102.779 | 48.656 | 32.390 | 1.00 | 36.27 |
| | 2498 | CD1 | TRP | 323 | 103.003 | 49.714 | 28.922 | 1.00 | 40.25 |
| | 2499 | NE1 | TRP | 323 | 104.312 | 49.500 | 29.286 | 1.00 | 39.37 |
| | 2500 | CZ2 | TRP | 323 | 105.439 | 48.753 | 31.402 | 1.00 | 30.80 |
| | 2501 | CZ3 | TRP | 323 | 103.863 | 48.322 | 33.192 | 1.00 | 34.06 |
| 10 | 2502 | CH2 | TRP | 323 | 105.178 | 48.374 | 32.691 | 1.00 | 37.92 |
| | 2503 | C | TRP | 323 | 100.182 | 51.976 | 29.606 | 1.00 | 36.88 |
| | 2504 | O | TRP | 323 | 100.522 | 51.788 | 28.437 | 1.00 | 30.80 |
| | 2505 | N | ASP | 324 | 99.781 | 53.157 | 30.066 | 1.00 | 48.71 |
| | 2506 | CA | ASP | 324 | 99.797 | 54.366 | 29.249 | 1.00 | 54.17 |
| | 2507 | CB | ASP | 324 | 98.462 | 54.586 | 28.537 | 1.00 | 56.16 |
| 15 | 2508 | CG | ASP | 324 | 98.585 | 55.547 | 27.366 | 1.00 | 58.43 |
| | 2509 | OD1 | ASP | 324 | 98.956 | 56.724 | 27.575 | 1.00 | 59.06 |
| | 2510 | OD2 | ASP | 324 | 98.328 | 55.120 | 26.222 | 1.00 | 57.24 |
| | 2511 | C | ASP | 324 | 100.076 | 55.543 | 30.165 | 1.00 | 57.09 |
| | 2512 | O | ASP | 324 | 99.468 | 55.671 | 31.230 | 1.00 | 54.89 |
| 20 | 2513 | N | ILE | 325 | 100.977 | 56.414 | 29.729 | 1.00 | 60.16 |
| | 2514 | CA | ILE | 325 | 101.377 | 57.584 | 30.495 | 1.00 | 64.12 |
| | 2515 | CB | ILE | 325 | 102.559 | 58.286 | 29.788 | 1.00 | 67.78 |
| | 2516 | CG2 | ILE | 325 | 102.072 | 59.013 | 28.542 | 1.00 | 68.84 |
| | 2517 | CG1 | ILE | 325 | 103.325 | 59.185 | 30.768 | 1.00 | 71.40 |
| 25 | 2518 | CD1 | ILE | 325 | 104.716 | 59.579 | 30.273 | 1.00 | 78.93 |
| | 2519 | C | ILE | 325 | 100.219 | 58.560 | 30.760 | 1.00 | 62.87 |
| | 2520 | O | ILE | 325 | 100.248 | 59.325 | 31.723 | 1.00 | 55.53 |
| | 2521 | N | ASN | 326 | 99.181 | 58.489 | 29.931 | 1.00 | 63.16 |
| | 2522 | CA | ASN | 326 | 98.008 | 59.347 | 30.075 | 1.00 | 60.43 |
| 30 | 2523 | CB | ASN | 326 | 97.060 | 59.157 | 28.891 | 1.00 | 58.85 |
| | 2524 | CG | ASN | 326 | 97.208 | 60.240 | 27.858 | 1.00 | 58.26 |
| | 2525 | OD1 | ASN | 326 | 97.005 | 61.420 | 28.150 | 1.00 | 61.96 |
| | 2526 | ND2 | ASN | 326 | 97.564 | 59.854 | 26.640 | 1.00 | 59.50 |
| | 2527 | C | ASN | 326 | 97.247 | 59.093 | 31.370 | 1.00 | 61.39 |
| 35 | 2528 | O | ASN | 326 | 96.561 | 59.982 | 31.875 | 1.00 | 62.82 |
| | 2529 | N | GLU | 327 | 97.378 | 57.881 | 31.904 | 1.00 | 59.66 |
| | 2530 | CA | GLU | 327 | 96.691 | 57.498 | 33.136 | 1.00 | 62.98 |
| | 2531 | CB | GLU | 327 | 96.563 | 55.973 | 33.216 | 1.00 | 64.39 |
| | 2532 | CG | GLU | 327 | 96.087 | 55.299 | 31.933 | 1.00 | 69.30 |
| 40 | 2533 | CD | GLU | 327 | 94.708 | 55.750 | 31.491 | 1.00 | 70.48 |
| | 2534 | OE1 | GLU | 327 | 93.784 | 55.783 | 32.335 | 1.00 | 72.78 |
| | 2535 | OE2 | GLU | 327 | 94.548 | 56.067 | 30.291 | 1.00 | 63.31 |
| | 2536 | C | GLU | 327 | 97.414 | 58.011 | 34.380 | 1.00 | 62.97 |
| | 2537 | O | GLU | 327 | 96.972 | 57.771 | 35.505 | 1.00 | 62.71 |
| 45 | 2538 | N | ILE | 328 | 98.510 | 58.734 | 34.169 | 1.00 | 64.24 |
| | 2539 | CA | ILE | 328 | 99.316 | 59.270 | 35.264 | 1.00 | 67.30 |
| | 2540 | CB | ILE | 328 | 100.636 | 59.886 | 34.729 | 1.00 | 69.70 |
| | 2541 | CG2 | ILE | 328 | 100.372 | 61.245 | 34.069 | 1.00 | 69.85 |
| | 2542 | CG1 | ILE | 328 | 101.657 | 60.013 | 35.863 | 1.00 | 72.49 |
| 50 | 2543 | CD1 | ILE | 328 | 103.047 | 60.424 | 35.409 | 1.00 | 71.67 |

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|----|------|-----|-----|-----|---------|--------|--------|------|--------|
| | 2544 | C | ILE | 328 | 98.577 | 60.298 | 36.122 | 1.00 | 66.37 |
| | 2545 | O | ILE | 328 | 98.763 | 60.349 | 37.340 | 1.00 | 61.63 |
| | 2546 | N | ASP | 329 | 97.711 | 61.082 | 35.485 | 1.00 | 70.35 |
| 5 | 2547 | CA | ASP | 329 | 96.950 | 62.128 | 36.163 | 1.00 | 73.14 |
| | 2548 | CB | ASP | 329 | 96.212 | 62.987 | 35.134 | 1.00 | 73.34 |
| | 2549 | CG | ASP | 329 | 97.154 | 63.620 | 34.123 | 1.00 | 75.99 |
| | 2550 | OD1 | ASP | 329 | 97.861 | 64.584 | 34.486 | 1.00 | 75.75 |
| | 2551 | OD2 | ASP | 329 | 97.198 | 63.140 | 32.970 | 1.00 | 74.82 |
| | 2552 | C | ASP | 329 | 95.978 | 61.611 | 37.219 | 1.00 | 73.26 |
| 10 | 2553 | O | ASP | 329 | 95.637 | 62.332 | 38.159 | 1.00 | 73.84 |
| | 2554 | N | ARG | 330 | 95.539 | 60.366 | 37.065 | 1.00 | 70.87 |
| | 2555 | CA | ARG | 330 | 94.616 | 59.756 | 38.019 | 1.00 | 70.53 |
| | 2556 | CB | ARG | 330 | 93.932 | 58.535 | 37.393 | 1.00 | 71.49 |
| | 2557 | CG | ARG | 330 | 93.145 | 58.845 | 36.129 | 1.00 | 78.19 |
| 15 | 2558 | CD | ARG | 330 | 92.435 | 57.612 | 35.591 | 1.00 | 85.11 |
| | 2559 | NE | ARG | 330 | 91.756 | 57.889 | 34.326 | 1.00 | 94.74 |
| | 2560 | CZ | ARG | 330 | 90.865 | 57.082 | 33.754 | 1.00 | 98.54 |
| | 2561 | NH1 | ARG | 330 | 90.532 | 55.934 | 34.331 | 1.00 | 100.00 |
| | 2562 | NH2 | ARG | 330 | 90.309 | 57.424 | 32.599 | 1.00 | 94.40 |
| 20 | 2563 | C | ARG | 330 | 95.358 | 59.345 | 39.291 | 1.00 | 67.20 |
| | 2564 | O | ARG | 330 | 94.749 | 59.145 | 40.345 | 1.00 | 61.95 |
| | 2565 | N | LEU | 331 | 96.681 | 59.252 | 39.183 | 1.00 | 66.11 |
| | 2566 | CA | LEU | 331 | 97.539 | 58.857 | 40.295 | 1.00 | 65.38 |
| | 2567 | CB | LEU | 331 | 98.727 | 58.047 | 39.768 | 1.00 | 70.15 |
| 25 | 2568 | CG | LEU | 331 | 98.430 | 56.802 | 38.933 | 1.00 | 71.98 |
| | 2569 | CD1 | LEU | 331 | 99.710 | 56.289 | 38.300 | 1.00 | 67.56 |
| | 2570 | CD2 | LEU | 331 | 97.789 | 55.739 | 39.806 | 1.00 | 72.35 |
| | 2571 | C | LEU | 331 | 98.081 | 60.056 | 41.057 | 1.00 | 59.96 |
| | 2572 | O | LEU | 331 | 98.432 | 61.069 | 40.456 | 1.00 | 60.57 |
| 30 | 2573 | N | PRO | 332 | 98.145 | 59.962 | 42.397 | 1.00 | 56.66 |
| | 2574 | CD | PRO | 332 | 97.661 | 58.870 | 43.257 | 1.00 | 52.18 |
| | 2575 | CA | PRO | 332 | 98.666 | 61.070 | 43.204 | 1.00 | 60.33 |
| | 2576 | CB | PRO | 332 | 98.458 | 60.578 | 44.640 | 1.00 | 54.14 |
| | 2577 | CG | PRO | 332 | 98.462 | 59.090 | 44.507 | 1.00 | 53.96 |
| 35 | 2578 | C | PRO | 332 | 100.144 | 61.294 | 42.871 | 1.00 | 65.03 |
| | 2579 | O | PRO | 332 | 100.817 | 60.386 | 42.381 | 1.00 | 68.68 |
| | 2580 | N | ASP | 333 | 100.637 | 62.500 | 43.136 | 1.00 | 70.86 |
| | 2581 | CA | ASP | 333 | 102.021 | 62.876 | 42.839 | 1.00 | 72.50 |
| | 2582 | CB | ASP | 333 | 102.362 | 64.220 | 43.489 | 1.00 | 76.30 |
| 40 | 2583 | CG | ASP | 333 | 101.737 | 65.396 | 42.760 | 1.00 | 73.02 |
| | 2584 | OD1 | ASP | 333 | 101.290 | 66.343 | 43.438 | 1.00 | 75.36 |
| | 2585 | OD2 | ASP | 333 | 101.700 | 65.378 | 41.510 | 1.00 | 70.83 |
| | 2586 | C | ASP | 333 | 103.146 | 61.873 | 43.105 | 1.00 | 69.45 |
| | 2587 | O | ASP | 333 | 104.019 | 61.694 | 42.254 | 1.00 | 64.53 |
| 45 | 2588 | N | TYR | 334 | 103.139 | 61.226 | 44.269 | 1.00 | 65.65 |
| | 2589 | CA | TYR | 334 | 104.195 | 60.267 | 44.590 | 1.00 | 64.14 |
| | 2590 | CB | TYR | 334 | 104.180 | 59.900 | 46.080 | 1.00 | 67.04 |
| | 2591 | CG | TYR | 334 | 103.162 | 58.858 | 46.484 | 1.00 | 71.84 |
| | 2592 | CD1 | TYR | 334 | 101.827 | 59.199 | 46.688 | 1.00 | 74.21 |
| 50 | 2593 | CE1 | TYR | 334 | 100.895 | 58.243 | 47.086 | 1.00 | 74.47 |

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|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 2594 | CD2 | TYR | 334 | 103.542 | 57.531 | 46.685 | 1.00 | 72.86 |
| | 2595 | CE2 | TYR | 334 | 102.620 | 56.570 | 47.081 | 1.00 | 72.07 |
| | 2596 | CZ | TYR | 334 | 101.299 | 56.932 | 47.281 | 1.00 | 72.74 |
| | 2597 | OH | TYR | 334 | 100.386 | 55.982 | 47.675 | 1.00 | 69.90 |
| 5 | 2598 | C | TYR | 334 | 104.143 | 59.015 | 43.714 | 1.00 | 59.49 |
| | 2599 | O | TYR | 334 | 105.181 | 58.466 | 43.341 | 1.00 | 58.89 |
| | 2600 | N | MET | 335 | 102.933 | 58.575 | 43.379 | 1.00 | 51.53 |
| | 2601 | CA | MET | 335 | 102.762 | 57.401 | 42.533 | 1.00 | 48.12 |
| | 2602 | CB | MET | 335 | 101.340 | 56.854 | 42.637 | 1.00 | 45.40 |
| 10 | 2603 | CG | MET | 335 | 100.979 | 56.325 | 44.006 | 1.00 | 34.82 |
| | 2604 | SD | MET | 335 | 99.387 | 55.502 | 44.005 | 1.00 | 37.30 |
| | 2605 | CE | MET | 335 | 99.776 | 53.994 | 44.867 | 1.00 | 41.41 |
| | 2606 | C | MET | 335 | 103.082 | 57.727 | 41.081 | 1.00 | 48.13 |
| | 2607 | O | MET | 335 | 103.354 | 56.826 | 40.287 | 1.00 | 55.57 |
| 15 | 2608 | N | LYS | 336 | 103.032 | 59.013 | 40.738 | 1.00 | 48.65 |
| | 2609 | CA | LYS | 336 | 103.332 | 59.465 | 39.380 | 1.00 | 50.84 |
| | 2610 | CB | LYS | 336 | 103.004 | 60.953 | 39.213 | 1.00 | 55.94 |
| | 2611 | CG | LYS | 336 | 101.524 | 61.301 | 39.255 | 1.00 | 63.40 |
| | 2612 | CD | LYS | 336 | 101.298 | 62.758 | 38.857 | 1.00 | 63.31 |
| 20 | 2613 | CE | LYS | 336 | 99.820 | 63.092 | 38.764 | 1.00 | 60.22 |
| | 2614 | NZ | LYS | 336 | 99.580 | 64.473 | 38.271 | 1.00 | 62.57 |
| | 2615 | C | LYS | 336 | 104.810 | 59.237 | 39.080 | 1.00 | 51.33 |
| | 2616 | O | LYS | 336 | 105.187 | 58.938 | 37.943 | 1.00 | 47.74 |
| 25 | 2617 | N | ILE | 337 | 105.638 | 59.382 | 40.114 | 1.00 | 45.10 |
| | 2618 | CA | ILE | 337 | 107.079 | 59.195 | 39.996 | 1.00 | 46.36 |
| | 2619 | CB | ILE | 337 | 107.805 | 59.607 | 41.297 | 1.00 | 48.91 |
| | 2620 | CG2 | ILE | 337 | 109.309 | 59.641 | 41.067 | 1.00 | 50.47 |
| | 2621 | CG1 | ILE | 337 | 107.330 | 60.986 | 41.759 | 1.00 | 50.88 |
| | 2622 | CD1 | ILE | 337 | 107.888 | 61.407 | 43.105 | 1.00 | 47.89 |
| 30 | 2623 | C | ILE | 337 | 107.380 | 57.725 | 39.712 | 1.00 | 47.32 |
| | 2624 | O | ILE | 337 | 108.140 | 57.402 | 38.795 | 1.00 | 52.27 |
| | 2625 | N | SER | 338 | 106.755 | 56.844 | 40.491 | 1.00 | 42.57 |
| | 2626 | CA | SER | 338 | 106.928 | 55.401 | 40.351 | 1.00 | 32.89 |
| | 2627 | CB | SER | 338 | 106.120 | 54.663 | 41.424 | 1.00 | 29.02 |
| 35 | 2628 | OG | SER | 338 | 106.339 | 55.198 | 42.718 | 1.00 | 33.47 |
| | 2629 | C | SER | 338 | 106.465 | 54.933 | 38.975 | 1.00 | 31.60 |
| | 2630 | O | SER | 338 | 107.214 | 54.287 | 38.243 | 1.00 | 27.59 |
| | 2631 | N | TYR | 339 | 105.239 | 55.311 | 38.621 | 1.00 | 33.89 |
| | 2632 | CA | TYR | 339 | 104.622 | 54.932 | 37.353 | 1.00 | 39.75 |
| 40 | 2633 | CB | TYR | 339 | 103.204 | 55.508 | 37.265 | 1.00 | 42.11 |
| | 2634 | CG | TYR | 339 | 102.367 | 54.908 | 36.157 | 1.00 | 46.50 |
| | 2635 | CD1 | TYR | 339 | 101.682 | 53.709 | 36.348 | 1.00 | 48.25 |
| | 2636 | CE1 | TYR | 339 | 100.924 | 53.144 | 35.327 | 1.00 | 52.79 |
| | 2637 | CD2 | TYR | 339 | 102.270 | 55.530 | 34.915 | 1.00 | 42.98 |
| 45 | 2638 | CE2 | TYR | 339 | 101.515 | 54.976 | 33.890 | 1.00 | 51.56 |
| | 2639 | CZ | TYR | 339 | 100.845 | 53.784 | 34.100 | 1.00 | 54.29 |
| | 2640 | OH | TYR | 339 | 100.100 | 53.236 | 33.080 | 1.00 | 56.73 |
| | 2641 | C | TYR | 339 | 105.414 | 55.309 | 36.101 | 1.00 | 43.13 |
| | 2642 | O | TYR | 339 | 105.531 | 54.502 | 35.174 | 1.00 | 41.07 |
| 50 | 2643 | N | LYS | 340 | 105.941 | 56.531 | 36.064 | 1.00 | 49.11 |

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|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 2644 | CA | LYS | 340 | 106.706 | 56.989 | 34.903 | 1.00 | 49.74 |
| | 2645 | CB | LYS | 340 | 106.894 | 58.508 | 34.934 | 1.00 | 58.08 |
| | 2646 | CG | LYS | 340 | 107.553 | 59.059 | 33.674 | 1.00 | 64.41 |
| | 2647 | CD | LYS | 340 | 107.642 | 60.573 | 33.694 | 1.00 | 69.77 |
| 5 | 2648 | CE | LYS | 340 | 108.246 | 61.097 | 32.403 | 1.00 | 73.44 |
| | 2649 | NZ | LYS | 340 | 108.256 | 62.584 | 32.365 | 1.00 | 82.14 |
| | 2650 | C | LYS | 340 | 108.062 | 56.297 | 34.800 | 1.00 | 44.71 |
| | 2651 | O | LYS | 340 | 108.506 | 55.938 | 33.703 | 1.00 | 34.93 |
| | 2652 | N | ALA | 341 | 108.712 | 56.114 | 35.948 | 1.00 | 36.45 |
| 10 | 2653 | CA | ALA | 341 | 110.013 | 55.456 | 36.003 | 1.00 | 36.97 |
| | 2654 | CB | ALA | 341 | 110.517 | 55.415 | 37.439 | 1.00 | 35.42 |
| | 2655 | C | ALA | 341 | 109.897 | 54.041 | 35.444 | 1.00 | 35.71 |
| | 2656 | O | ALA | 341 | 110.791 | 53.561 | 34.746 | 1.00 | 34.74 |
| | 2657 | N | ILE | 342 | 108.766 | 53.399 | 35.734 | 1.00 | 29.99 |
| 15 | 2658 | CA | ILE | 342 | 108.487 | 52.041 | 35.283 | 1.00 | 21.08 |
| | 2659 | CB | ILE | 342 | 107.231 | 51.472 | 35.982 | 1.00 | 16.81 |
| | 2660 | CG2 | ILE | 342 | 106.786 | 50.171 | 35.309 | 1.00 | 10.96 |
| | 2661 | CG1 | ILE | 342 | 107.523 | 51.275 | 37.476 | 1.00 | 10.78 |
| | 2662 | CD1 | ILE | 342 | 106.333 | 50.884 | 38.324 | 1.00 | 2.00 |
| 20 | 2663 | C | ILE | 342 | 108.336 | 51.939 | 33.771 | 1.00 | 28.67 |
| | 2664 | O | ILE | 342 | 108.949 | 51.071 | 33.150 | 1.00 | 32.50 |
| | 2665 | N | LEU | 343 | 107.530 | 52.821 | 33.180 | 1.00 | 33.81 |
| | 2666 | CA | LEU | 343 | 107.320 | 52.809 | 31.732 | 1.00 | 37.97 |
| | 2667 | CB | LEU | 343 | 106.208 | 53.774 | 31.317 | 1.00 | 41.50 |
| 25 | 2668 | CG | LEU | 343 | 104.822 | 53.594 | 31.932 | 1.00 | 46.77 |
| | 2669 | CD1 | LEU | 343 | 103.831 | 54.537 | 31.267 | 1.00 | 48.11 |
| | 2670 | CD2 | LEU | 343 | 104.375 | 52.165 | 31.759 | 1.00 | 43.32 |
| | 2671 | C | LEU | 343 | 108.596 | 53.177 | 30.995 | 1.00 | 41.41 |
| | 2672 | O | LEU | 343 | 108.880 | 52.626 | 29.932 | 1.00 | 43.16 |
| 30 | 2673 | N | ASP | 344 | 109.348 | 54.126 | 31.552 | 1.00 | 45.08 |
| | 2674 | CA | ASP | 344 | 110.601 | 54.563 | 30.942 | 1.00 | 51.08 |
| | 2675 | CB | ASP | 344 | 111.144 | 55.820 | 31.628 | 1.00 | 57.96 |
| | 2676 | CG | ASP | 344 | 110.754 | 57.098 | 30.903 | 1.00 | 64.16 |
| | 2677 | OD1 | ASP | 344 | 110.680 | 57.090 | 29.654 | 1.00 | 69.36 |
| 35 | 2678 | OD2 | ASP | 344 | 110.526 | 58.117 | 31.588 | 1.00 | 65.04 |
| | 2679 | C | ASP | 344 | 111.643 | 53.461 | 30.980 | 1.00 | 50.69 |
| | 2680 | O | ASP | 344 | 112.415 | 53.301 | 30.034 | 1.00 | 53.80 |
| | 2681 | N | LEU | 345 | 111.661 | 52.709 | 32.078 | 1.00 | 47.98 |
| | 2682 | CA | LEU | 345 | 112.594 | 51.599 | 32.242 | 1.00 | 43.23 |
| 40 | 2683 | CB | LEU | 345 | 112.384 | 50.925 | 33.599 | 1.00 | 45.16 |
| | 2684 | CG | LEU | 345 | 113.317 | 49.773 | 33.977 | 1.00 | 44.62 |
| | 2685 | CD1 | LEU | 345 | 114.752 | 50.267 | 34.070 | 1.00 | 45.63 |
| | 2686 | CD2 | LEU | 345 | 112.875 | 49.186 | 35.307 | 1.00 | 42.33 |
| | 2687 | C | LEU | 345 | 112.364 | 50.585 | 31.129 | 1.00 | 42.19 |
| 45 | 2688 | O | LEU | 345 | 113.315 | 50.068 | 30.541 | 1.00 | 47.47 |
| | 2689 | N | TYR | 346 | 111.094 | 50.311 | 30.844 | 1.00 | 38.09 |
| | 2690 | CA | TYR | 346 | 110.731 | 49.372 | 29.793 | 1.00 | 36.61 |
| | 2691 | CB | TYR | 346 | 109.298 | 48.878 | 29.983 | 1.00 | 32.28 |
| | 2692 | CG | TYR | 346 | 109.211 | 47.802 | 31.038 | 1.00 | 30.73 |
| 50 | 2693 | CD1 | TYR | 346 | 108.903 | 48.110 | 32.361 | 1.00 | 22.11 |

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|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 2694 | CE1 | TYR | 346 | 108.895 | 47.122 | 33.346 | 1.00 | 24.69 |
| | 2695 | CD2 | TYR | 346 | 109.503 | 46.477 | 30.722 | 1.00 | 35.15 |
| | 2696 | CE2 | TYR | 346 | 109.499 | 45.484 | 31.694 | 1.00 | 26.34 |
| | 2697 | CZ | TYR | 346 | 109.198 | 45.809 | 33.000 | 1.00 | 27.54 |
| 5 | 2698 | OH | TYR | 346 | 109.224 | 44.812 | 33.948 | 1.00 | 22.51 |
| | 2699 | C | TYR | 346 | 110.954 | 49.953 | 28.403 | 1.00 | 39.45 |
| | 2700 | O | TYR | 346 | 111.086 | 49.213 | 27.429 | 1.00 | 37.79 |
| | 2701 | N | LYS | 347 | 110.995 | 51.281 | 28.320 | 1.00 | 44.42 |
| | 2702 | CA | LYS | 347 | 111.256 | 51.958 | 27.056 | 1.00 | 45.72 |
| 10 | 2703 | CB | LYS | 347 | 110.797 | 53.418 | 27.105 | 1.00 | 49.09 |
| | 2704 | CG | LYS | 347 | 109.313 | 53.604 | 26.824 | 1.00 | 54.73 |
| | 2705 | CD | LYS | 347 | 108.959 | 53.084 | 25.433 | 1.00 | 58.88 |
| | 2706 | CE | LYS | 347 | 107.471 | 53.195 | 25.149 | 1.00 | 58.70 |
| | 2707 | NZ | LYS | 347 | 107.129 | 52.632 | 23.816 | 1.00 | 45.34 |
| 15 | 2708 | C | LYS | 347 | 112.756 | 51.874 | 26.810 | 1.00 | 44.56 |
| | 2709 | O | LYS | 347 | 113.201 | 51.803 | 25.666 | 1.00 | 44.20 |
| | 2710 | N | ASP | 348 | 113.524 | 51.865 | 27.901 | 1.00 | 45.25 |
| | 2711 | CA | ASP | 348 | 114.977 | 51.748 | 27.829 | 1.00 | 43.43 |
| | 2712 | CB | ASP | 348 | 115.630 | 52.041 | 29.188 | 1.00 | 41.08 |
| 20 | 2713 | CG | ASP | 348 | 115.545 | 53.509 | 29.584 | 1.00 | 45.56 |
| | 2714 | OD1 | ASP | 348 | 115.741 | 54.388 | 28.716 | 1.00 | 50.29 |
| | 2715 | OD2 | ASP | 348 | 115.293 | 53.787 | 30.775 | 1.00 | 46.84 |
| | 2716 | C | ASP | 348 | 115.308 | 50.325 | 27.394 | 1.00 | 44.57 |
| | 2717 | O | ASP | 348 | 116.186 | 50.116 | 26.555 | 1.00 | 45.03 |
| 25 | 2718 | N | TYR | 349 | 114.585 | 49.355 | 27.959 | 1.00 | 43.55 |
| | 2719 | CA | TYR | 349 | 114.773 | 47.943 | 27.627 | 1.00 | 42.30 |
| | 2720 | CB | TYR | 349 | 113.813 | 47.054 | 28.429 | 1.00 | 41.29 |
| | 2721 | CG | TYR | 349 | 114.128 | 46.916 | 29.906 | 1.00 | 37.24 |
| | 2722 | CD1 | TYR | 349 | 113.181 | 46.393 | 30.785 | 1.00 | 30.06 |
| 30 | 2723 | CE1 | TYR | 349 | 113.458 | 46.247 | 32.142 | 1.00 | 36.46 |
| | 2724 | CD2 | TYR | 349 | 115.368 | 47.293 | 30.424 | 1.00 | 41.76 |
| | 2725 | CE2 | TYR | 349 | 115.656 | 47.151 | 31.783 | 1.00 | 40.50 |
| | 2726 | CZ | TYR | 349 | 114.694 | 46.627 | 32.633 | 1.00 | 36.99 |
| | 2727 | OH | TYR | 349 | 114.960 | 46.491 | 33.975 | 1.00 | 36.59 |
| 35 | 2728 | C | TYR | 349 | 114.520 | 47.741 | 26.139 | 1.00 | 42.51 |
| | 2729 | O | TYR | 349 | 115.308 | 47.094 | 25.446 | 1.00 | 42.03 |
| | 2730 | N | GLU | 350 | 113.411 | 48.296 | 25.656 | 1.00 | 44.24 |
| | 2731 | CA | GLU | 350 | 113.053 | 48.199 | 24.244 | 1.00 | 46.89 |
| | 2732 | CB | GLU | 350 | 111.734 | 48.929 | 23.969 | 1.00 | 49.81 |
| 40 | 2733 | CG | GLU | 350 | 110.509 | 48.270 | 24.589 | 1.00 | 54.69 |
| | 2734 | CD | GLU | 350 | 109.214 | 49.033 | 24.347 | 1.00 | 58.54 |
| | 2735 | OE1 | GLU | 350 | 108.144 | 48.491 | 24.695 | 1.00 | 62.24 |
| | 2736 | OE2 | GLU | 350 | 109.253 | 50.168 | 23.822 | 1.00 | 64.71 |
| | 2737 | C | GLU | 350 | 114.162 | 48.811 | 23.397 | 1.00 | 48.29 |
| 45 | 2738 | O | GLU | 350 | 114.491 | 48.294 | 22.334 | 1.00 | 45.94 |
| | 2739 | N | LYS | 351 | 114.763 | 49.884 | 23.909 | 1.00 | 53.89 |
| | 2740 | CA | LYS | 351 | 115.841 | 50.591 | 23.222 | 1.00 | 58.14 |
| | 2741 | CB | LYS | 351 | 116.053 | 51.971 | 23.855 | 1.00 | 63.43 |
| | 2742 | CG | LYS | 351 | 116.916 | 52.921 | 23.031 | 1.00 | 71.72 |
| 50 | 2743 | CD | LYS | 351 | 116.247 | 53.286 | 21.711 | 1.00 | 77.97 |

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|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 2744 | CE | LYS | 351 | 117.122 | 54.218 | 20.885 | 1.00 | 83.68 |
| | 2745 | NZ | LYS | 351 | 116.483 | 54.588 | 19.591 | 1.00 | 83.73 |
| | 2746 | C | LYS | 351 | 117.155 | 49.795 | 23.215 | 1.00 | 57.54 |
| | 2747 | O | LYS | 351 | 117.873 | 49.784 | 22.209 | 1.00 | 56.27 |
| 5 | 2748 | N | GLU | 352 | 117.465 | 49.142 | 24.336 | 1.00 | 56.46 |
| | 2749 | CA | GLU | 352 | 118.684 | 48.334 | 24.458 | 1.00 | 52.60 |
| | 2750 | CB | GLU | 352 | 118.847 | 47.801 | 25.890 | 1.00 | 50.25 |
| | 2751 | CG | GLU | 352 | 119.239 | 48.828 | 26.943 | 1.00 | 58.10 |
| | 2752 | CD | GLU | 352 | 119.464 | 48.194 | 28.311 | 1.00 | 59.00 |
| 10 | 2753 | OE1 | GLU | 352 | 118.655 | 48.447 | 29.232 | 1.00 | 57.55 |
| | 2754 | OE2 | GLU | 352 | 120.447 | 47.435 | 28.468 | 1.00 | 53.94 |
| | 2755 | C | GLU | 352 | 118.645 | 47.140 | 23.508 | 1.00 | 49.57 |
| | 2756 | O | GLU | 352 | 119.671 | 46.735 | 22.957 | 1.00 | 45.55 |
| | 2757 | N | LEU | 353 | 117.448 | 46.587 | 23.327 | 1.00 | 44.88 |
| 15 | 2758 | CA | LEU | 353 | 117.239 | 45.432 | 22.463 | 1.00 | 44.80 |
| | 2759 | CB | LEU | 353 | 116.116 | 44.561 | 23.034 | 1.00 | 35.61 |
| | 2760 | CG | LEU | 353 | 116.304 | 44.125 | 24.489 | 1.00 | 30.68 |
| | 2761 | CD1 | LEU | 353 | 115.030 | 43.507 | 25.030 | 1.00 | 31.93 |
| | 2762 | CD2 | LEU | 353 | 117.468 | 43.156 | 24.597 | 1.00 | 32.93 |
| 20 | 2763 | C | LEU | 353 | 116.937 | 45.806 | 21.011 | 1.00 | 48.25 |
| | 2764 | O | LEU | 353 | 116.878 | 44.933 | 20.140 | 1.00 | 48.95 |
| | 2765 | N | SER | 354 | 116.756 | 47.101 | 20.751 | 1.00 | 54.12 |
| | 2766 | CA | SER | 354 | 116.468 | 47.595 | 19.403 | 1.00 | 58.83 |
| | 2767 | CB | SER | 354 | 116.356 | 49.122 | 19.395 | 1.00 | 64.47 |
| 25 | 2768 | OG | SER | 354 | 115.196 | 49.571 | 20.072 | 1.00 | 73.04 |
| | 2769 | C | SER | 354 | 117.534 | 47.171 | 18.400 | 1.00 | 58.85 |
| | 2770 | O | SER | 354 | 117.226 | 46.900 | 17.237 | 1.00 | 60.25 |
| | 2771 | N | SER | 355 | 118.784 | 47.119 | 18.857 | 1.00 | 59.55 |
| | 2772 | CA | SER | 355 | 119.918 | 46.731 | 18.022 | 1.00 | 60.93 |
| 30 | 2773 | CB | SER | 355 | 121.219 | 46.840 | 18.823 | 1.00 | 58.82 |
| | 2774 | OG | SER | 355 | 122.333 | 46.392 | 18.071 | 1.00 | 61.05 |
| | 2775 | C | SER | 355 | 119.772 | 45.316 | 17.455 | 1.00 | 67.50 |
| | 2776 | O | SER | 355 | 119.753 | 45.125 | 16.239 | 1.00 | 72.60 |
| | 2777 | N | ALA | 356 | 119.640 | 44.338 | 18.345 | 1.00 | 68.57 |
| 35 | 2778 | CA | ALA | 356 | 119.501 | 42.943 | 17.946 | 1.00 | 67.55 |
| | 2779 | CB | ALA | 356 | 119.690 | 42.040 | 19.152 | 1.00 | 63.74 |
| | 2780 | C | ALA | 356 | 118.163 | 42.642 | 17.278 | 1.00 | 69.18 |
| | 2781 | O | ALA | 356 | 118.071 | 41.754 | 16.434 | 1.00 | 70.23 |
| | 2782 | N | GLY | 357 | 117.131 | 43.385 | 17.661 | 1.00 | 69.13 |
| 40 | 2783 | CA | GLY | 357 | 115.811 | 43.152 | 17.102 | 1.00 | 62.21 |
| | 2784 | C | GLY | 357 | 115.027 | 42.258 | 18.039 | 1.00 | 59.93 |
| | 2785 | O | GLY | 357 | 114.203 | 41.443 | 17.604 | 1.00 | 60.71 |
| | 2786 | N | ARG | 358 | 115.322 | 42.391 | 19.332 | 1.00 | 54.34 |
| | 2787 | CA | ARG | 358 | 114.669 | 41.616 | 20.385 | 1.00 | 52.71 |
| 45 | 2788 | CB | ARG | 358 | 115.713 | 40.882 | 21.231 | 1.00 | 45.26 |
| | 2789 | CG | ARG | 358 | 116.561 | 39.896 | 20.442 | 1.00 | 47.78 |
| | 2790 | CD | ARG | 358 | 117.644 | 39.275 | 21.309 | 1.00 | 47.12 |
| | 2791 | NE | ARG | 358 | 117.083 | 38.456 | 22.383 | 1.00 | 44.42 |
| | 2792 | CZ | ARG | 358 | 117.206 | 38.724 | 23.681 | 1.00 | 39.46 |
| 50 | 2793 | NH1 | ARG | 358 | 117.871 | 39.797 | 24.083 | 1.00 | 37.90 |

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|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 2794 | NH2 | ARG | 358 | 116.684 | 37.905 | 24.583 | 1.00 | 43.78 |
| | 2795 | C | ARG | 358 | 113.817 | 42.522 | 21.282 | 1.00 | 55.62 |
| | 2796 | O | ARG | 358 | 113.676 | 42.268 | 22.479 | 1.00 | 60.74 |
| 5 | 2797 | N | SER | 359 | 113.286 | 43.596 | 20.699 | 1.00 | 54.17 |
| | 2798 | CA | SER | 359 | 112.440 | 44.548 | 21.419 | 1.00 | 49.75 |
| | 2799 | CB | SER | 359 | 112.373 | 45.887 | 20.671 | 1.00 | 46.10 |
| | 2800 | OG | SER | 359 | 113.659 | 46.424 | 20.441 | 1.00 | 39.24 |
| | 2801 | C | SER | 359 | 111.030 | 43.979 | 21.584 | 1.00 | 51.35 |
| | 2802 | O | SER | 359 | 110.321 | 44.294 | 22.549 | 1.00 | 51.03 |
| 10 | 2803 | N | HIS | 360 | 110.642 | 43.145 | 20.619 | 1.00 | 48.18 |
| | 2804 | CA | HIS | 360 | 109.339 | 42.484 | 20.566 | 1.00 | 49.55 |
| | 2805 | CB | HIS | 360 | 109.165 | 41.769 | 19.214 | 1.00 | 55.45 |
| | 2806 | CG | HIS | 360 | 110.191 | 40.706 | 18.955 | 1.00 | 57.94 |
| | 2807 | CD2 | HIS | 360 | 111.485 | 40.791 | 18.565 | 1.00 | 58.70 |
| 15 | 2808 | ND1 | HIS | 360 | 109.933 | 39.363 | 19.134 | 1.00 | 62.62 |
| | 2809 | CE1 | HIS | 360 | 111.028 | 38.668 | 18.875 | 1.00 | 63.83 |
| | 2810 | NE2 | HIS | 360 | 111.985 | 39.511 | 18.527 | 1.00 | 63.77 |
| | 2811 | C | HIS | 360 | 109.105 | 41.483 | 21.705 | 1.00 | 51.67 |
| | 2812 | O | HIS | 360 | 108.023 | 40.886 | 21.795 | 1.00 | 56.00 |
| 20 | 2813 | N | ILE | 361 | 110.115 | 41.294 | 22.552 | 1.00 | 44.35 |
| | 2814 | CA | ILE | 361 | 110.005 | 40.352 | 23.659 | 1.00 | 40.02 |
| | 2815 | CB | ILE | 361 | 111.217 | 39.396 | 23.719 | 1.00 | 40.34 |
| | 2816 | CG2 | ILE | 361 | 111.350 | 38.631 | 22.412 | 1.00 | 38.81 |
| | 2817 | CG1 | ILE | 361 | 112.490 | 40.174 | 24.052 | 1.00 | 45.99 |
| 25 | 2818 | CD1 | ILE | 361 | 113.742 | 39.324 | 24.096 | 1.00 | 38.31 |
| | 2819 | C | ILE | 361 | 109.837 | 41.012 | 25.022 | 1.00 | 38.58 |
| | 2820 | O | ILE | 361 | 109.629 | 40.323 | 26.018 | 1.00 | 46.53 |
| | 2821 | N | VAL | 362 | 109.920 | 42.339 | 25.068 | 1.00 | 34.37 |
| | 2822 | CA | VAL | 362 | 109.784 | 43.073 | 26.323 | 1.00 | 36.05 |
| 30 | 2823 | CB | VAL | 362 | 110.133 | 44.567 | 26.131 | 1.00 | 44.38 |
| | 2824 | CG1 | VAL | 362 | 110.157 | 45.290 | 27.474 | 1.00 | 28.09 |
| | 2825 | CG2 | VAL | 362 | 111.470 | 44.705 | 25.420 | 1.00 | 50.90 |
| | 2826 | C | VAL | 362 | 108.372 | 42.959 | 26.899 | 1.00 | 35.07 |
| | 2827 | O | VAL | 362 | 108.187 | 43.012 | 28.113 | 1.00 | 27.77 |
| 35 | 2828 | N | CYS | 363 | 107.383 | 42.770 | 26.025 | 1.00 | 37.13 |
| | 2829 | CA | CYS | 363 | 105.980 | 42.653 | 26.437 | 1.00 | 34.16 |
| | 2830 | CB | CYS | 363 | 105.066 | 42.483 | 25.215 | 1.00 | 29.73 |
| | 2831 | SG | CYS | 363 | 105.447 | 41.051 | 24.179 | 1.00 | 41.96 |
| | 2832 | C | CYS | 363 | 105.730 | 41.520 | 27.434 | 1.00 | 32.61 |
| 40 | 2833 | O | CYS | 363 | 104.887 | 41.646 | 28.325 | 1.00 | 25.38 |
| | 2834 | N | HIS | 364 | 106.481 | 40.429 | 27.292 | 1.00 | 28.31 |
| | 2835 | CA | HIS | 364 | 106.356 | 39.267 | 28.168 | 1.00 | 20.38 |
| | 2836 | CB | HIS | 364 | 107.304 | 38.159 | 27.713 | 1.00 | 19.91 |
| | 2837 | CG | HIS | 364 | 107.064 | 37.696 | 26.309 | 1.00 | 25.64 |
| 45 | 2838 | CD2 | HIS | 364 | 107.777 | 37.887 | 25.173 | 1.00 | 29.90 |
| | 2839 | ND1 | HIS | 364 | 105.976 | 36.929 | 25.954 | 1.00 | 34.65 |
| | 2840 | CE1 | HIS | 364 | 106.028 | 36.667 | 24.659 | 1.00 | 33.79 |
| | 2841 | NE2 | HIS | 364 | 107.111 | 37.237 | 24.162 | 1.00 | 27.05 |
| | 2842 | C | HIS | 364 | 106.646 | 39.635 | 29.622 | 1.00 | 28.17 |
| 50 | 2843 | O | HIS | 364 | 105.942 | 39.200 | 30.537 | 1.00 | 27.54 |

| | | | | | | | | | |
|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 2844 | N | ALA | 365 | 107.685 | 40.440 | 29.826 | 1.00 | 30.22 |
| | 2845 | CA | ALA | 365 | 108.067 | 40.880 | 31.163 | 1.00 | 30.86 |
| | 2846 | CB | ALA | 365 | 109.427 | 41.574 | 31.120 | 1.00 | 34.60 |
| | 2847 | C | ALA | 365 | 107.007 | 41.822 | 31.725 | 1.00 | 31.03 |
| 5 | 2848 | O | ALA | 365 | 106.752 | 41.838 | 32.931 | 1.00 | 31.19 |
| | 2849 | N | ILE | 366 | 106.389 | 42.596 | 30.835 | 1.00 | 36.30 |
| | 2850 | CA | ILE | 366 | 105.347 | 43.550 | 31.208 | 1.00 | 36.55 |
| | 2851 | CB | ILE | 366 | 105.016 | 44.504 | 30.034 | 1.00 | 41.23 |
| | 2852 | CG2 | ILE | 366 | 103.857 | 45.419 | 30.403 | 1.00 | 40.62 |
| 10 | 2853 | CG1 | ILE | 366 | 106.253 | 45.331 | 29.668 | 1.00 | 35.62 |
| | 2854 | CD1 | ILE | 366 | 106.065 | 46.231 | 28.468 | 1.00 | 29.32 |
| | 2855 | C | ILE | 366 | 104.070 | 42.845 | 31.667 | 1.00 | 30.85 |
| | 2856 | O | ILE | 366 | 103.524 | 43.173 | 32.722 | 1.00 | 28.50 |
| | 2857 | N | GLU | 367 | 103.613 | 41.867 | 30.886 | 1.00 | 25.21 |
| 15 | 2858 | CA | GLU | 367 | 102.404 | 41.117 | 31.223 | 1.00 | 22.77 |
| | 2859 | CB | GLU | 367 | 102.095 | 40.069 | 30.153 | 1.00 | 32.06 |
| | 2860 | CG | GLU | 367 | 101.926 | 40.626 | 28.736 | 1.00 | 41.69 |
| | 2861 | CD | GLU | 367 | 100.870 | 41.721 | 28.629 | 1.00 | 48.62 |
| | 2862 | OE1 | GLU | 367 | 99.829 | 41.633 | 29.321 | 1.00 | 48.68 |
| 20 | 2863 | OE2 | GLU | 367 | 101.083 | 42.670 | 27.841 | 1.00 | 43.16 |
| | 2864 | C | GLU | 367 | 102.539 | 40.448 | 32.585 | 1.00 | 20.02 |
| | 2865 | O | GLU | 367 | 101.555 | 40.297 | 33.314 | 1.00 | 20.91 |
| | 2866 | N | ARG | 368 | 103.766 | 40.057 | 32.923 | 1.00 | 21.53 |
| | 2867 | CA | ARG | 368 | 104.055 | 39.422 | 34.205 | 1.00 | 14.50 |
| 25 | 2868 | CB | ARG | 368 | 105.406 | 38.709 | 34.159 | 1.00 | 17.59 |
| | 2869 | CG | ARG | 368 | 105.427 | 37.442 | 33.319 | 1.00 | 13.40 |
| | 2870 | CD | ARG | 368 | 104.602 | 36.338 | 33.960 | 1.00 | 17.58 |
| | 2871 | NE | ARG | 368 | 104.843 | 35.044 | 33.325 | 1.00 | 25.37 |
| | 2872 | CZ | ARG | 368 | 104.380 | 33.884 | 33.784 | 1.00 | 29.88 |
| 30 | 2873 | NH1 | ARG | 368 | 103.641 | 33.847 | 34.887 | 1.00 | 15.72 |
| | 2874 | NH2 | ARG | 368 | 104.669 | 32.757 | 33.146 | 1.00 | 25.60 |
| | 2875 | C | ARG | 368 | 104.058 | 40.473 | 35.306 | 1.00 | 22.28 |
| | 2876 | O | ARG | 368 | 103.674 | 40.193 | 36.444 | 1.00 | 25.28 |
| | 2877 | N | MET | 369 | 104.489 | 41.686 | 34.965 | 1.00 | 23.23 |
| 35 | 2878 | CA | MET | 369 | 104.513 | 42.774 | 35.933 | 1.00 | 22.69 |
| | 2879 | CB | MET | 369 | 105.234 | 44.001 | 35.371 | 1.00 | 21.94 |
| | 2880 | CG | MET | 369 | 105.216 | 45.178 | 36.332 | 1.00 | 33.04 |
| | 2881 | SD | MET | 369 | 106.226 | 46.580 | 35.855 | 1.00 | 30.05 |
| | 2882 | CE | MET | 369 | 106.788 | 47.105 | 37.492 | 1.00 | 22.46 |
| 40 | 2883 | C | MET | 369 | 103.088 | 43.138 | 36.329 | 1.00 | 21.30 |
| | 2884 | O | MET | 369 | 102.794 | 43.316 | 37.513 | 1.00 | 25.30 |
| | 2885 | N | LYS | 370 | 102.207 | 43.230 | 35.332 | 1.00 | 22.42 |
| | 2886 | CA | LYS | 370 | 100.798 | 43.555 | 35.562 | 1.00 | 21.17 |
| | 2887 | CB | LYS | 370 | 100.033 | 43.596 | 34.237 | 1.00 | 18.37 |
| 45 | 2888 | CG | LYS | 370 | 100.498 | 44.679 | 33.272 | 1.00 | 19.38 |
| | 2889 | CD | LYS | 370 | 99.724 | 44.628 | 31.959 | 1.00 | 22.90 |
| | 2890 | CE | LYS | 370 | 100.144 | 45.754 | 31.026 | 1.00 | 25.30 |
| | 2891 | NZ | LYS | 370 | 99.370 | 45.760 | 29.753 | 1.00 | 26.14 |
| | 2892 | C | LYS | 370 | 100.184 | 42.503 | 36.480 | 1.00 | 22.60 |
| 50 | 2893 | O | LYS | 370 | 99.433 | 42.830 | 37.404 | 1.00 | 22.82 |

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|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 2894 | N | GLU | 371 | 100.540 | 41.243 | 36.233 | 1.00 | 20.87 |
| | 2895 | CA | GLU | 371 | 100.060 | 40.117 | 37.027 | 1.00 | 17.91 |
| | 2896 | CB | GLU | 371 | 100.633 | 38.805 | 36.473 | 1.00 | 17.04 |
| 5 | 2897 | CG | GLU | 371 | 100.291 | 37.558 | 37.281 | 1.00 | 14.89 |
| | 2898 | CD | GLU | 371 | 100.951 | 36.307 | 36.737 | 1.00 | 33.96 |
| | 2899 | OE1 | GLU | 371 | 100.246 | 35.281 | 36.624 | 1.00 | 49.48 |
| | 2900 | OE2 | GLU | 371 | 102.162 | 36.342 | 36.433 | 1.00 | 39.35 |
| | 2901 | C | GLU | 371 | 100.459 | 40.291 | 38.491 | 1.00 | 14.70 |
| | 2902 | O | GLU | 371 | 99.629 | 40.146 | 39.389 | 1.00 | 15.00 |
| 10 | 2903 | N | VAL | 372 | 101.727 | 40.624 | 38.718 | 1.00 | 16.52 |
| | 2904 | CA | VAL | 372 | 102.246 | 40.830 | 40.066 | 1.00 | 17.45 |
| | 2905 | CB | VAL | 372 | 103.747 | 41.232 | 40.043 | 1.00 | 17.58 |
| | 2906 | CG1 | VAL | 372 | 104.258 | 41.453 | 41.450 | 1.00 | 3.56 |
| | 2907 | CG2 | VAL | 372 | 104.575 | 40.156 | 39.365 | 1.00 | 18.80 |
| 15 | 2908 | C | VAL | 372 | 101.455 | 41.919 | 40.782 | 1.00 | 21.27 |
| | 2909 | O | VAL | 372 | 101.101 | 41.767 | 41.952 | 1.00 | 23.46 |
| | 2910 | N | VAL | 373 | 101.155 | 43.000 | 40.063 | 1.00 | 26.12 |
| | 2911 | CA | VAL | 373 | 100.407 | 44.123 | 40.629 | 1.00 | 29.37 |
| | 2912 | CB | VAL | 373 | 100.425 | 45.356 | 39.694 | 1.00 | 33.84 |
| 20 | 2913 | CG1 | VAL | 373 | 99.736 | 46.537 | 40.366 | 1.00 | 27.54 |
| | 2914 | CG2 | VAL | 373 | 101.861 | 45.724 | 39.335 | 1.00 | 29.76 |
| | 2915 | C | VAL | 373 | 98.962 | 43.754 | 40.969 | 1.00 | 29.64 |
| | 2916 | O | VAL | 373 | 98.462 | 44.135 | 42.030 | 1.00 | 27.43 |
| | 2917 | N | ARG | 374 | 98.298 | 43.015 | 40.078 | 1.00 | 27.06 |
| 25 | 2918 | CA | ARG | 374 | 96.916 | 42.587 | 40.315 | 1.00 | 22.92 |
| | 2919 | CB | ARG | 374 | 96.438 | 41.626 | 39.225 | 1.00 | 20.10 |
| | 2920 | CG | ARG | 374 | 96.101 | 42.257 | 37.897 | 1.00 | 18.80 |
| | 2921 | CD | ARG | 374 | 95.627 | 41.191 | 36.924 | 1.00 | 11.40 |
| | 2922 | NE | ARG | 374 | 96.410 | 41.194 | 35.692 | 1.00 | 20.17 |
| 30 | 2923 | CZ | ARG | 374 | 96.956 | 40.112 | 35.146 | 1.00 | 19.94 |
| | 2924 | NH1 | ARG | 374 | 96.810 | 38.924 | 35.720 | 1.00 | 26.31 |
| | 2925 | NH2 | ARG | 374 | 97.655 | 40.218 | 34.025 | 1.00 | 24.45 |
| | 2926 | C | ARG | 374 | 96.835 | 41.858 | 41.646 | 1.00 | 26.89 |
| | 2927 | O | ARG | 374 | 95.964 | 42.134 | 42.472 | 1.00 | 32.47 |
| 35 | 2928 | N | ASN | 375 | 97.766 | 40.931 | 41.842 | 1.00 | 27.68 |
| | 2929 | CA | ASN | 375 | 97.827 | 40.133 | 43.055 | 1.00 | 25.57 |
| | 2930 | CB | ASN | 375 | 98.776 | 38.955 | 42.850 | 1.00 | 30.36 |
| | 2931 | CG | ASN | 375 | 98.299 | 38.009 | 41.756 | 1.00 | 32.94 |
| | 2932 | OD1 | ASN | 375 | 97.594 | 38.415 | 40.827 | 1.00 | 25.76 |
| 40 | 2933 | ND2 | ASN | 375 | 98.677 | 36.741 | 41.865 | 1.00 | 30.37 |
| | 2934 | C | ASN | 375 | 98.213 | 40.958 | 44.279 | 1.00 | 26.96 |
| | 2935 | O | ASN | 375 | 97.819 | 40.632 | 45.399 | 1.00 | 21.31 |
| | 2936 | N | TYR | 376 | 98.980 | 42.026 | 44.062 | 1.00 | 33.99 |
| | 2937 | CA | TYR | 376 | 99.381 | 42.920 | 45.148 | 1.00 | 33.87 |
| 45 | 2938 | CB | TYR | 376 | 100.362 | 43.986 | 44.645 | 1.00 | 39.17 |
| | 2939 | CG | TYR | 376 | 101.823 | 43.579 | 44.628 | 1.00 | 42.30 |
| | 2940 | CD1 | TYR | 376 | 102.765 | 44.344 | 43.940 | 1.00 | 40.53 |
| | 2941 | CE1 | TYR | 376 | 104.111 | 43.997 | 43.934 | 1.00 | 45.46 |
| | 2942 | CD2 | TYR | 376 | 102.268 | 42.446 | 45.312 | 1.00 | 43.05 |
| 50 | 2943 | CE2 | TYR | 376 | 103.614 | 42.088 | 45.313 | 1.00 | 42.63 |

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|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 2944 | CZ | TYR | 376 | 104.531 | 42.868 | 44.623 | 1.00 | 48.37 |
| | 2945 | OH | TYR | 376 | 105.865 | 42.523 | 44.621 | 1.00 | 39.23 |
| | 2946 | C | TYR | 376 | 98.122 | 43.605 | 45.668 | 1.00 | 29.88 |
| | 2947 | O | TYR | 376 | 97.942 | 43.773 | 46.874 | 1.00 | 27.89 |
| 5 | 2948 | N | ASN | 377 | 97.252 | 43.984 | 44.733 | 1.00 | 29.64 |
| | 2949 | CA | ASN | 377 | 95.987 | 44.642 | 45.043 | 1.00 | 31.75 |
| | 2950 | CB | ASN | 377 | 95.304 | 45.094 | 43.748 | 1.00 | 34.90 |
| | 2951 | CG | ASN | 377 | 94.116 | 45.999 | 43.999 | 1.00 | 40.49 |
| | 2952 | OD1 | ASN | 377 | 92.992 | 45.532 | 44.178 | 1.00 | 42.59 |
| 10 | 2953 | ND2 | ASN | 377 | 94.360 | 47.303 | 44.011 | 1.00 | 34.81 |
| | 2954 | C | ASN | 377 | 95.084 | 43.674 | 45.804 | 1.00 | 28.41 |
| | 2955 | O | ASN | 377 | 94.538 | 44.015 | 46.857 | 1.00 | 30.58 |
| | 2956 | N | VAL | 378 | 94.952 | 42.460 | 45.274 | 1.00 | 17.90 |
| | 2957 | CA | VAL | 378 | 94.131 | 41.426 | 45.900 | 1.00 | 17.33 |
| 15 | 2958 | CB | VAL | 378 | 94.186 | 40.112 | 45.086 | 1.00 | 10.51 |
| | 2959 | CG1 | VAL | 378 | 93.423 | 39.012 | 45.789 | 1.00 | 11.35 |
| | 2960 | CG2 | VAL | 378 | 93.612 | 40.332 | 43.698 | 1.00 | 13.48 |
| | 2961 | C | VAL | 378 | 94.616 | 41.163 | 47.327 | 1.00 | 25.35 |
| | 2962 | O | VAL | 378 | 93.813 | 40.997 | 48.248 | 1.00 | 27.43 |
| 20 | 2963 | N | GLU | 379 | 95.936 | 41.176 | 47.497 | 1.00 | 31.20 |
| | 2964 | CA | GLU | 379 | 96.575 | 40.938 | 48.787 | 1.00 | 33.04 |
| | 2965 | CB | GLU | 379 | 98.100 | 40.924 | 48.613 | 1.00 | 40.56 |
| | 2966 | CG | GLU | 379 | 98.888 | 40.454 | 49.836 | 1.00 | 52.37 |
| | 2967 | CD | GLU | 379 | 100.392 | 40.399 | 49.591 | 1.00 | 57.31 |
| 25 | 2968 | OE1 | GLU | 379 | 101.158 | 40.762 | 50.510 | 1.00 | 59.83 |
| | 2969 | OE2 | GLU | 379 | 100.810 | 39.986 | 48.485 | 1.00 | 55.53 |
| | 2970 | C | GLU | 379 | 96.166 | 41.984 | 49.825 | 1.00 | 31.53 |
| | 2971 | O | GLU | 379 | 95.922 | 41.650 | 50.987 | 1.00 | 29.16 |
| | 2972 | N | SER | 380 | 96.092 | 43.245 | 49.402 | 1.00 | 32.96 |
| 30 | 2973 | CA | SER | 380 | 95.706 | 44.331 | 50.300 | 1.00 | 37.42 |
| | 2974 | CB | SER | 380 | 96.066 | 45.695 | 49.698 | 1.00 | 38.70 |
| | 2975 | OG | SER | 380 | 95.348 | 45.945 | 48.504 | 1.00 | 49.17 |
| | 2976 | C | SER | 380 | 94.212 | 44.264 | 50.604 | 1.00 | 38.16 |
| | 2977 | O | SER | 380 | 93.789 | 44.512 | 51.737 | 1.00 | 31.46 |
| 35 | 2978 | N | THR | 381 | 93.424 | 43.915 | 49.587 | 1.00 | 36.08 |
| | 2979 | CA | THR | 381 | 91.976 | 43.790 | 49.729 | 1.00 | 27.53 |
| | 2980 | CB | THR | 381 | 91.320 | 43.333 | 48.413 | 1.00 | 22.85 |
| | 2981 | OG1 | THR | 381 | 91.706 | 44.212 | 47.350 | 1.00 | 16.53 |
| | 2982 | CG2 | THR | 381 | 89.812 | 43.351 | 48.543 | 1.00 | 23.91 |
| 40 | 2983 | C | THR | 381 | 91.662 | 42.762 | 50.814 | 1.00 | 27.68 |
| | 2984 | O | THR | 381 | 90.813 | 42.996 | 51.670 | 1.00 | 29.54 |
| | 2985 | N | TRP | 382 | 92.375 | 41.637 | 50.779 | 1.00 | 28.31 |
| | 2986 | CA | TRP | 382 | 92.199 | 40.563 | 51.755 | 1.00 | 28.12 |
| | 2987 | CB | TRP | 382 | 93.063 | 39.353 | 51.386 | 1.00 | 36.50 |
| 45 | 2988 | CG | TRP | 382 | 92.583 | 38.570 | 50.195 | 1.00 | 38.50 |
| | 2989 | CD2 | TRP | 382 | 93.258 | 37.475 | 49.565 | 1.00 | 42.33 |
| | 2990 | CE2 | TRP | 382 | 92.430 | 37.022 | 48.516 | 1.00 | 44.37 |
| | 2991 | CE3 | TRP | 382 | 94.483 | 36.830 | 49.787 | 1.00 | 47.90 |
| | 2992 | CD1 | TRP | 382 | 91.408 | 38.735 | 49.518 | 1.00 | 36.49 |
| 50 | 2993 | NE1 | TRP | 382 | 91.308 | 37.808 | 48.511 | 1.00 | 36.31 |

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|----|------|-----|-----|-----|--------|--------|--------|------|-------|
| | 2994 | CZ2 | TRP | 382 | 92.787 | 35.951 | 47.688 | 1.00 | 51.17 |
| | 2995 | CZ3 | TRP | 382 | 94.838 | 35.764 | 48.963 | 1.00 | 43.35 |
| | 2996 | CH2 | TRP | 382 | 93.991 | 35.337 | 47.927 | 1.00 | 45.79 |
| | 2997 | C | TRP | 382 | 92.567 | 41.030 | 53.157 | 1.00 | 30.09 |
| 5 | 2998 | O | TRP | 382 | 91.926 | 40.651 | 54.137 | 1.00 | 31.61 |
| | 2999 | N | PHE | 383 | 93.617 | 41.841 | 53.240 | 1.00 | 36.62 |
| | 3000 | CA | PHE | 383 | 94.092 | 42.378 | 54.510 | 1.00 | 38.24 |
| | 3001 | CB | PHE | 383 | 95.411 | 43.138 | 54.298 | 1.00 | 36.46 |
| | 3002 | CG | PHE | 383 | 95.885 | 43.880 | 55.516 | 1.00 | 32.91 |
| 10 | 3003 | CD1 | PHE | 383 | 96.157 | 43.202 | 56.701 | 1.00 | 32.24 |
| | 3004 | CD2 | PHE | 383 | 96.020 | 45.264 | 55.490 | 1.00 | 33.47 |
| | 3005 | CE1 | PHE | 383 | 96.553 | 43.892 | 57.843 | 1.00 | 34.44 |
| | 3006 | CE2 | PHE | 383 | 96.415 | 45.963 | 56.628 | 1.00 | 34.81 |
| | 3007 | CZ | PHE | 383 | 96.681 | 45.275 | 57.807 | 1.00 | 35.83 |
| 15 | 3008 | C | PHE | 383 | 93.045 | 43.296 | 55.144 | 1.00 | 38.45 |
| | 3009 | O | PHE | 383 | 92.793 | 43.223 | 56.351 | 1.00 | 36.37 |
| | 3010 | N | ILE | 384 | 92.436 | 44.144 | 54.315 | 1.00 | 36.46 |
| | 3011 | CA | ILE | 384 | 91.410 | 45.091 | 54.756 | 1.00 | 34.56 |
| | 3012 | CB | ILE | 384 | 91.025 | 46.062 | 53.615 | 1.00 | 27.26 |
| 20 | 3013 | CG2 | ILE | 384 | 89.917 | 46.996 | 54.066 | 1.00 | 33.92 |
| | 3014 | CG1 | ILE | 384 | 92.249 | 46.870 | 53.171 | 1.00 | 30.39 |
| | 3015 | CD1 | ILE | 384 | 92.881 | 47.691 | 54.278 | 1.00 | 31.10 |
| | 3016 | C | ILE | 384 | 90.145 | 44.391 | 55.255 | 1.00 | 34.50 |
| | 3017 | O | ILE | 384 | 89.634 | 44.702 | 56.333 | 1.00 | 36.61 |
| 25 | 3018 | N | GLU | 385 | 89.643 | 43.453 | 54.460 | 1.00 | 26.50 |
| | 3019 | CA | GLU | 385 | 88.443 | 42.703 | 54.811 | 1.00 | 26.95 |
| | 3020 | CB | GLU | 385 | 87.937 | 41.926 | 53.595 | 1.00 | 21.63 |
| | 3021 | CG | GLU | 385 | 87.650 | 42.790 | 52.375 | 1.00 | 29.50 |
| | 3022 | CD | GLU | 385 | 87.418 | 41.976 | 51.115 | 1.00 | 38.78 |
| 30 | 3023 | OE1 | GLU | 385 | 87.706 | 40.758 | 51.124 | 1.00 | 42.45 |
| | 3024 | OE2 | GLU | 385 | 86.955 | 42.560 | 50.110 | 1.00 | 36.35 |
| | 3025 | C | GLU | 385 | 88.711 | 41.732 | 55.954 | 1.00 | 32.21 |
| | 3026 | O | GLU | 385 | 87.778 | 41.289 | 56.629 | 1.00 | 43.97 |
| | 3027 | N | GLY | 386 | 89.985 | 41.419 | 56.184 | 1.00 | 30.98 |
| 35 | 3028 | CA | GLY | 386 | 90.341 | 40.486 | 57.238 | 1.00 | 29.71 |
| | 3029 | C | GLY | 386 | 90.069 | 39.071 | 56.767 | 1.00 | 29.59 |
| | 3030 | O | GLY | 386 | 89.738 | 38.178 | 57.557 | 1.00 | 27.61 |
| | 3031 | N | TYR | 387 | 90.238 | 38.877 | 55.461 | 1.00 | 23.79 |
| | 3032 | CA | TYR | 387 | 89.999 | 37.595 | 54.816 | 1.00 | 27.24 |
| 40 | 3033 | CB | TYR | 387 | 89.744 | 37.802 | 53.319 | 1.00 | 29.04 |
| | 3034 | CG | TYR | 387 | 89.248 | 36.570 | 52.580 | 1.00 | 23.98 |
| | 3035 | CD1 | TYR | 387 | 88.361 | 35.675 | 53.179 | 1.00 | 22.30 |
| | 3036 | CE1 | TYR | 387 | 87.891 | 34.552 | 52.493 | 1.00 | 29.04 |
| | 3037 | CD2 | TYR | 387 | 89.657 | 36.311 | 51.271 | 1.00 | 26.35 |
| 45 | 3038 | CE2 | TYR | 387 | 89.192 | 35.194 | 50.575 | 1.00 | 24.90 |
| | 3039 | CZ | TYR | 387 | 88.311 | 34.320 | 51.191 | 1.00 | 29.66 |
| | 3040 | OH | TYR | 387 | 87.848 | 33.218 | 50.510 | 1.00 | 26.42 |
| | 3041 | C | TYR | 387 | 91.127 | 36.591 | 55.014 | 1.00 | 30.82 |
| | 3042 | O | TYR | 387 | 92.311 | 36.917 | 54.874 | 1.00 | 39.13 |
| 50 | 3043 | N | THR | 388 | 90.721 | 35.375 | 55.364 | 1.00 | 37.65 |

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|----|------|-----|-----|-----|--------|--------|--------|------|-------|
| | 3044 | CA | THR | 388 | 91.623 | 34.247 | 55.568 | 1.00 | 31.40 |
| | 3045 | CB | THR | 388 | 91.576 | 33.728 | 57.025 | 1.00 | 33.01 |
| | 3046 | OG1 | THR | 388 | 92.090 | 34.729 | 57.911 | 1.00 | 35.43 |
| | 3047 | CG2 | THR | 388 | 92.416 | 32.462 | 57.179 | 1.00 | 38.16 |
| 5 | 3048 | C | THR | 388 | 91.140 | 33.148 | 54.609 | 1.00 | 31.72 |
| | 3049 | O | THR | 388 | 90.343 | 32.282 | 54.981 | 1.00 | 39.68 |
| | 3050 | N | PRO | 389 | 91.581 | 33.203 | 53.335 | 1.00 | 25.34 |
| | 3051 | CD | PRO | 389 | 92.494 | 34.204 | 52.755 | 1.00 | 23.99 |
| | 3052 | CA | PRO | 389 | 91.190 | 32.214 | 52.323 | 1.00 | 26.01 |
| 10 | 3053 | CB | PRO | 389 | 91.717 | 32.829 | 51.030 | 1.00 | 21.95 |
| | 3054 | CG | PRO | 389 | 92.953 | 33.531 | 51.475 | 1.00 | 17.85 |
| | 3055 | C | PRO | 389 | 91.779 | 30.825 | 52.537 | 1.00 | 30.44 |
| | 3056 | O | PRO | 389 | 92.711 | 30.651 | 53.324 | 1.00 | 28.62 |
| | 3057 | N | PRO | 390 | 91.177 | 29.805 | 51.909 | 1.00 | 32.36 |
| 15 | 3058 | CD | PRO | 390 | 89.921 | 29.814 | 51.135 | 1.00 | 26.81 |
| | 3059 | CA | PRO | 390 | 91.691 | 28.442 | 52.047 | 1.00 | 33.56 |
| | 3060 | CB | PRO | 390 | 90.600 | 27.601 | 51.379 | 1.00 | 32.56 |
| | 3061 | CG | PRO | 390 | 90.024 | 28.532 | 50.356 | 1.00 | 23.42 |
| | 3062 | C | PRO | 390 | 93.016 | 28.383 | 51.277 | 1.00 | 34.49 |
| 20 | 3063 | O | PRO | 390 | 93.222 | 29.160 | 50.335 | 1.00 | 30.76 |
| | 3064 | N | VAL | 391 | 93.920 | 27.494 | 51.689 | 1.00 | 29.65 |
| | 3065 | CA | VAL | 391 | 95.230 | 27.360 | 51.046 | 1.00 | 25.79 |
| | 3066 | CB | VAL | 391 | 95.943 | 26.061 | 51.479 | 1.00 | 23.80 |
| | 3067 | CG1 | VAL | 391 | 97.314 | 25.969 | 50.831 | 1.00 | 20.24 |
| 25 | 3068 | CG2 | VAL | 391 | 96.078 | 26.017 | 52.981 | 1.00 | 16.75 |
| | 3069 | C | VAL | 391 | 95.155 | 27.393 | 49.523 | 1.00 | 25.32 |
| | 3070 | O | VAL | 391 | 95.944 | 28.075 | 48.868 | 1.00 | 27.66 |
| | 3071 | N | SER | 392 | 94.178 | 26.683 | 48.970 | 1.00 | 25.00 |
| | 3072 | CA | SER | 392 | 93.993 | 26.621 | 47.527 | 1.00 | 25.90 |
| 30 | 3073 | CB | SER | 392 | 92.727 | 25.827 | 47.194 | 1.00 | 26.67 |
| | 3074 | OG | SER | 392 | 92.570 | 25.684 | 45.794 | 1.00 | 47.32 |
| | 3075 | C | SER | 392 | 93.911 | 28.015 | 46.918 | 1.00 | 18.85 |
| | 3076 | O | SER | 392 | 94.671 | 28.350 | 46.011 | 1.00 | 19.28 |
| | 3077 | N | GLU | 393 | 93.013 | 28.837 | 47.450 | 1.00 | 16.74 |
| 35 | 3078 | CA | GLU | 393 | 92.827 | 30.191 | 46.949 | 1.00 | 24.04 |
| | 3079 | CB | GLU | 393 | 91.579 | 30.821 | 47.565 | 1.00 | 27.67 |
| | 3080 | CG | GLU | 393 | 91.105 | 32.067 | 46.831 | 1.00 | 20.67 |
| | 3081 | CD | GLU | 393 | 90.095 | 32.873 | 47.618 | 1.00 | 19.63 |
| | 3082 | OE1 | GLU | 393 | 89.550 | 32.362 | 48.619 | 1.00 | 20.04 |
| 40 | 3083 | OE2 | GLU | 393 | 89.853 | 34.032 | 47.232 | 1.00 | 26.17 |
| | 3084 | C | GLU | 393 | 94.044 | 31.071 | 47.226 | 1.00 | 27.53 |
| | 3085 | O | GLU | 393 | 94.474 | 31.837 | 46.361 | 1.00 | 22.89 |
| | 3086 | N | TYR | 394 | 94.590 | 30.960 | 48.435 | 1.00 | 26.05 |
| | 3087 | CA | TYR | 394 | 95.762 | 31.736 | 48.829 | 1.00 | 26.22 |
| 45 | 3088 | CB | TYR | 394 | 96.252 | 31.293 | 50.211 | 1.00 | 32.15 |
| | 3089 | CG | TYR | 394 | 97.597 | 31.868 | 50.595 | 1.00 | 37.24 |
| | 3090 | CD1 | TYR | 394 | 97.739 | 33.224 | 50.890 | 1.00 | 37.33 |
| | 3091 | CE1 | TYR | 394 | 98.980 | 33.762 | 51.214 | 1.00 | 33.89 |
| | 3092 | CD2 | TYR | 394 | 98.733 | 31.061 | 50.639 | 1.00 | 35.64 |
| 50 | 3093 | CE2 | TYR | 394 | 99.979 | 31.590 | 50.961 | 1.00 | 31.95 |

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|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 3094 | CZ | TYR | 394 | 100.095 | 32.941 | 51.248 | 1.00 | 34.89 |
| | 3095 | OH | TYR | 394 | 101.324 | 33.471 | 51.562 | 1.00 | 35.44 |
| | 3096 | C | TYR | 394 | 96.900 | 31.615 | 47.813 | 1.00 | 27.71 |
| | 3097 | O | TYR | 394 | 97.400 | 32.622 | 47.310 | 1.00 | 30.17 |
| 5 | 3098 | N | LEU | 395 | 97.278 | 30.379 | 47.496 | 1.00 | 19.47 |
| | 3099 | CA | LEU | 395 | 98.356 | 30.112 | 46.551 | 1.00 | 18.70 |
| | 3100 | CB | LEU | 395 | 98.664 | 28.615 | 46.506 | 1.00 | 23.07 |
| | 3101 | CG | LEU | 395 | 99.219 | 28.005 | 47.796 | 1.00 | 25.20 |
| | 3102 | CD1 | LEU | 395 | 99.416 | 26.512 | 47.609 | 1.00 | 19.35 |
| 10 | 3103 | CD2 | LEU | 395 | 100.532 | 28.681 | 48.180 | 1.00 | 17.74 |
| | 3104 | C | LEU | 395 | 98.106 | 30.630 | 45.140 | 1.00 | 19.62 |
| | 3105 | O | LEU | 395 | 99.030 | 31.112 | 44.485 | 1.00 | 19.16 |
| | 3106 | N | SER | 396 | 96.862 | 30.549 | 44.676 | 1.00 | 25.13 |
| | 3107 | CA | SER | 396 | 96.521 | 31.018 | 43.332 | 1.00 | 19.88 |
| 15 | 3108 | CB | SER | 396 | 95.047 | 30.749 | 43.022 | 1.00 | 25.09 |
| | 3109 | OG | SER | 396 | 94.196 | 31.513 | 43.858 | 1.00 | 39.87 |
| | 3110 | C | SER | 396 | 96.828 | 32.504 | 43.165 | 1.00 | 19.03 |
| | 3111 | O | SER | 396 | 96.920 | 33.005 | 42.040 | 1.00 | 15.70 |
| | 3112 | N | ASN | 397 | 96.999 | 33.198 | 44.290 | 1.00 | 14.51 |
| 20 | 3113 | CA | ASN | 397 | 97.308 | 34.624 | 44.281 | 1.00 | 20.25 |
| | 3114 | CB | ASN | 397 | 96.252 | 35.401 | 45.072 | 1.00 | 21.33 |
| | 3115 | CG | ASN | 397 | 96.348 | 36.901 | 44.858 | 1.00 | 25.70 |
| | 3116 | OD1 | ASN | 397 | 95.985 | 37.411 | 43.795 | 1.00 | 26.44 |
| | 3117 | ND2 | ASN | 397 | 96.840 | 37.617 | 45.868 | 1.00 | 14.18 |
| 25 | 3118 | C | ASN | 397 | 98.702 | 34.926 | 44.844 | 1.00 | 21.44 |
| | 3119 | O | ASN | 397 | 99.446 | 35.727 | 44.277 | 1.00 | 16.68 |
| | 3120 | N | ALA | 398 | 99.053 | 34.263 | 45.944 | 1.00 | 21.43 |
| | 3121 | CA | ALA | 398 | 100.339 | 34.463 | 46.611 | 1.00 | 18.24 |
| | 3122 | CB | ALA | 398 | 100.303 | 33.853 | 47.996 | 1.00 | 9.21 |
| 30 | 3123 | C | ALA | 398 | 101.576 | 33.973 | 45.861 | 1.00 | 22.03 |
| | 3124 | O | ALA | 398 | 102.693 | 34.375 | 46.183 | 1.00 | 27.40 |
| | 3125 | N | LEU | 399 | 101.392 | 33.099 | 44.878 | 1.00 | 24.29 |
| | 3126 | CA | LEU | 399 | 102.530 | 32.590 | 44.123 | 1.00 | 21.14 |
| | 3127 | CB | LEU | 399 | 102.133 | 31.379 | 43.276 | 1.00 | 16.51 |
| 35 | 3128 | CG | LEU | 399 | 101.814 | 30.092 | 44.047 | 1.00 | 22.47 |
| | 3129 | CD1 | LEU | 399 | 101.475 | 28.979 | 43.068 | 1.00 | 23.59 |
| | 3130 | CD2 | LEU | 399 | 102.986 | 29.686 | 44.929 | 1.00 | 24.50 |
| | 3131 | C | LEU | 399 | 103.189 | 33.656 | 43.256 | 1.00 | 21.08 |
| | 3132 | O | LEU | 399 | 104.414 | 33.724 | 43.181 | 1.00 | 27.40 |
| 40 | 3133 | N | ALA | 400 | 102.384 | 34.499 | 42.618 | 1.00 | 23.35 |
| | 3134 | CA | ALA | 400 | 102.921 | 35.556 | 41.762 | 1.00 | 25.45 |
| | 3135 | CB | ALA | 400 | 101.860 | 36.050 | 40.782 | 1.00 | 20.16 |
| | 3136 | C | ALA | 400 | 103.500 | 36.724 | 42.562 | 1.00 | 21.72 |
| | 3137 | O | ALA | 400 | 104.438 | 37.380 | 42.109 | 1.00 | 16.17 |
| 45 | 3138 | N | THR | 401 | 102.960 | 36.966 | 43.757 | 1.00 | 16.96 |
| | 3139 | CA | THR | 401 | 103.445 | 38.054 | 44.605 | 1.00 | 19.18 |
| | 3140 | CB | THR | 401 | 102.535 | 38.294 | 45.832 | 1.00 | 15.54 |
| | 3141 | OG1 | THR | 401 | 102.407 | 37.090 | 46.592 | 1.00 | 24.65 |
| | 3142 | CG2 | THR | 401 | 101.167 | 38.752 | 45.393 | 1.00 | 12.23 |
| 50 | 3143 | C | THR | 401 | 104.893 | 37.842 | 45.055 | 1.00 | 25.46 |

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|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 3144 | O | THR | 401 | 105.512 | 38.743 | 45.624 | 1.00 | 34.91 |
| | 3145 | N | THR | 402 | 105.421 | 36.644 | 44.813 | 1.00 | 25.90 |
| | 3146 | CA | THR | 402 | 106.807 | 36.336 | 45.151 | 1.00 | 21.29 |
| | 3147 | CB | THR | 402 | 107.092 | 34.812 | 45.138 | 1.00 | 19.71 |
| 5 | 3148 | OG1 | THR | 402 | 106.944 | 34.300 | 43.806 | 1.00 | 12.44 |
| | 3149 | CG2 | THR | 402 | 106.152 | 34.080 | 46.070 | 1.00 | 17.92 |
| | 3150 | C | THR | 402 | 107.674 | 36.988 | 44.076 | 1.00 | 22.11 |
| | 3151 | O | THR | 402 | 108.881 | 37.135 | 44.245 | 1.00 | 21.20 |
| 10 | 3152 | N | THR | 403 | 107.022 | 37.366 | 42.974 | 1.00 | 21.28 |
| | 3153 | CA | THR | 403 | 107.629 | 38.010 | 41.804 | 1.00 | 18.85 |
| | 3154 | CB | THR | 403 | 108.446 | 39.288 | 42.167 | 1.00 | 15.80 |
| | 3155 | OG1 | THR | 403 | 109.662 | 38.922 | 42.827 | 1.00 | 16.98 |
| | 3156 | CG2 | THR | 403 | 107.647 | 40.210 | 43.071 | 1.00 | 14.55 |
| | 3157 | C | THR | 403 | 108.515 | 37.084 | 40.980 | 1.00 | 17.52 |
| 15 | 3158 | O | THR | 403 | 109.136 | 37.523 | 40.013 | 1.00 | 14.77 |
| | 3159 | N | TYR | 404 | 108.533 | 35.799 | 41.326 | 1.00 | 19.57 |
| | 3160 | CA | TYR | 404 | 109.375 | 34.842 | 40.617 | 1.00 | 16.03 |
| | 3161 | CB | TYR | 404 | 109.560 | 33.560 | 41.431 | 1.00 | 23.52 |
| | 3162 | CG | TYR | 404 | 110.799 | 33.611 | 42.295 | 1.00 | 19.00 |
| 20 | 3163 | CD1 | TYR | 404 | 111.271 | 34.828 | 42.785 | 1.00 | 20.18 |
| | 3164 | CE1 | TYR | 404 | 112.430 | 34.903 | 43.536 | 1.00 | 26.20 |
| | 3165 | CD2 | TYR | 404 | 111.527 | 32.459 | 42.586 | 1.00 | 21.26 |
| | 3166 | CE2 | TYR | 404 | 112.695 | 32.523 | 43.345 | 1.00 | 26.60 |
| | 3167 | CZ | TYR | 404 | 113.139 | 33.753 | 43.813 | 1.00 | 25.95 |
| 25 | 3168 | OH | TYR | 404 | 114.291 | 33.853 | 44.553 | 1.00 | 17.83 |
| | 3169 | C | TYR | 404 | 109.040 | 34.545 | 39.164 | 1.00 | 16.09 |
| | 3170 | O | TYR | 404 | 109.945 | 34.265 | 38.375 | 1.00 | 15.20 |
| | 3171 | N | TYR | 405 | 107.760 | 34.593 | 38.803 | 1.00 | 14.07 |
| 30 | 3172 | CA | TYR | 405 | 107.375 | 34.360 | 37.411 | 1.00 | 18.64 |
| | 3173 | CB | TYR | 405 | 105.852 | 34.353 | 37.250 | 1.00 | 21.43 |
| | 3174 | CG | TYR | 405 | 105.096 | 33.276 | 37.991 | 1.00 | 14.20 |
| | 3175 | CD1 | TYR | 405 | 104.458 | 33.557 | 39.196 | 1.00 | 25.61 |
| | 3176 | CE1 | TYR | 405 | 103.687 | 32.599 | 39.844 | 1.00 | 26.54 |
| | 3177 | CD2 | TYR | 405 | 104.949 | 31.998 | 37.452 | 1.00 | 18.03 |
| 35 | 3178 | CE2 | TYR | 405 | 104.178 | 31.031 | 38.094 | 1.00 | 15.71 |
| | 3179 | CZ | TYR | 405 | 103.550 | 31.341 | 39.290 | 1.00 | 17.50 |
| | 3180 | OH | TYR | 405 | 102.785 | 30.404 | 39.941 | 1.00 | 14.13 |
| | 3181 | C | TYR | 405 | 107.922 | 35.558 | 36.638 | 1.00 | 16.83 |
| | 3182 | O | TYR | 405 | 108.450 | 35.433 | 35.532 | 1.00 | 12.99 |
| 40 | 3183 | N | TYR | 406 | 107.784 | 36.718 | 37.271 | 1.00 | 19.05 |
| | 3184 | CA | TYR | 406 | 108.213 | 38.005 | 36.749 | 1.00 | 20.07 |
| | 3185 | CB | TYR | 406 | 107.708 | 39.095 | 37.709 | 1.00 | 20.76 |
| | 3186 | CG | TYR | 406 | 108.060 | 40.523 | 37.365 | 1.00 | 13.44 |
| | 3187 | CD1 | TYR | 406 | 108.092 | 40.965 | 36.044 | 1.00 | 16.24 |
| 45 | 3188 | CE1 | TYR | 406 | 108.412 | 42.284 | 35.739 | 1.00 | 19.34 |
| | 3189 | CD2 | TYR | 406 | 108.355 | 41.436 | 38.373 | 1.00 | 2.00 |
| | 3190 | CE2 | TYR | 406 | 108.673 | 42.751 | 38.081 | 1.00 | 7.86 |
| | 3191 | CZ | TYR | 406 | 108.701 | 43.171 | 36.764 | 1.00 | 14.60 |
| | 3192 | OH | TYR | 406 | 109.015 | 44.481 | 36.481 | 1.00 | 12.74 |
| 50 | 3193 | C | TYR | 406 | 109.735 | 38.068 | 36.570 | 1.00 | 18.51 |

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|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 3194 | O | TYR | 406 | 110.222 | 38.302 | 35.462 | 1.00 | 20.47 |
| | 3195 | N | LEU | 407 | 110.478 | 37.822 | 37.647 | 1.00 | 18.49 |
| | 3196 | CA | LEU | 407 | 111.944 | 37.854 | 37.602 | 1.00 | 17.48 |
| | 3197 | CB | LEU | 407 | 112.536 | 37.617 | 38.994 | 1.00 | 9.18 |
| 5 | 3198 | CG | LEU | 407 | 112.066 | 38.535 | 40.125 | 1.00 | 11.41 |
| | 3199 | CD1 | LEU | 407 | 112.894 | 38.261 | 41.366 | 1.00 | 4.35 |
| | 3200 | CD2 | LEU | 407 | 112.179 | 40.001 | 39.714 | 1.00 | 14.20 |
| | 3201 | C | LEU | 407 | 112.533 | 36.843 | 36.619 | 1.00 | 17.93 |
| | 3202 | O | LEU | 407 | 113.506 | 37.142 | 35.925 | 1.00 | 23.70 |
| 10 | 3203 | N | ALA | 408 | 111.944 | 35.650 | 36.568 | 1.00 | 17.24 |
| | 3204 | CA | ALA | 408 | 112.402 | 34.603 | 35.662 | 1.00 | 15.77 |
| | 3205 | CB | ALA | 408 | 111.636 | 33.320 | 35.913 | 1.00 | 20.39 |
| | 3206 | C | ALA | 408 | 112.233 | 35.046 | 34.214 | 1.00 | 15.32 |
| | 3207 | O | ALA | 408 | 113.108 | 34.820 | 33.383 | 1.00 | 19.31 |
| 15 | 3208 | N | THR | 409 | 111.106 | 35.685 | 33.919 | 1.00 | 18.97 |
| | 3209 | CA | THR | 409 | 110.830 | 36.174 | 32.570 | 1.00 | 20.42 |
| | 3210 | CB | THR | 409 | 109.382 | 36.705 | 32.455 | 1.00 | 12.64 |
| | 3211 | OG1 | THR | 409 | 108.465 | 35.679 | 32.853 | 1.00 | 23.03 |
| | 3212 | CG2 | THR | 409 | 109.074 | 37.116 | 31.023 | 1.00 | 8.86 |
| 20 | 3213 | C | THR | 409 | 111.804 | 37.302 | 32.233 | 1.00 | 18.76 |
| | 3214 | O | THR | 409 | 112.269 | 37.426 | 31.096 | 1.00 | 14.71 |
| | 3215 | N | THR | 410 | 112.118 | 38.105 | 33.245 | 1.00 | 23.19 |
| | 3216 | CA | THR | 410 | 113.031 | 39.232 | 33.105 | 1.00 | 22.03 |
| | 3217 | CB | THR | 410 | 113.060 | 40.078 | 34.390 | 1.00 | 17.23 |
| 25 | 3218 | OG1 | THR | 410 | 111.751 | 40.600 | 34.652 | 1.00 | 20.47 |
| | 3219 | CG2 | THR | 410 | 114.043 | 41.228 | 34.251 | 1.00 | 18.91 |
| | 3220 | C | THR | 410 | 114.453 | 38.781 | 32.790 | 1.00 | 25.12 |
| | 3221 | O | THR | 410 | 115.109 | 39.356 | 31.918 | 1.00 | 24.94 |
| | 3222 | N | SER | 411 | 114.913 | 37.741 | 33.486 | 1.00 | 18.76 |
| 30 | 3223 | CA | SER | 411 | 116.264 | 37.221 | 33.298 | 1.00 | 11.15 |
| | 3224 | CB | SER | 411 | 116.517 | 36.026 | 34.224 | 1.00 | 9.23 |
| | 3225 | OG | SER | 411 | 115.722 | 34.911 | 33.871 | 1.00 | 10.06 |
| | 3226 | C | SER | 411 | 116.586 | 36.859 | 31.848 | 1.00 | 15.22 |
| | 3227 | O | SER | 411 | 117.744 | 36.915 | 31.431 | 1.00 | 22.78 |
| 35 | 3228 | N | TYR | 412 | 115.555 | 36.525 | 31.078 | 1.00 | 12.29 |
| | 3229 | CA | TYR | 412 | 115.715 | 36.165 | 29.673 | 1.00 | 14.56 |
| | 3230 | CB | TYR | 412 | 114.473 | 35.428 | 29.160 | 1.00 | 21.66 |
| | 3231 | CG | TYR | 412 | 114.284 | 34.000 | 29.630 | 1.00 | 31.85 |
| | 3232 | CD1 | TYR | 412 | 113.510 | 33.110 | 28.884 | 1.00 | 25.46 |
| 40 | 3233 | CE1 | TYR | 412 | 113.285 | 31.807 | 29.315 | 1.00 | 25.33 |
| | 3234 | CD2 | TYR | 412 | 114.837 | 33.544 | 30.829 | 1.00 | 33.63 |
| | 3235 | CE2 | TYR | 412 | 114.617 | 32.236 | 31.271 | 1.00 | 30.87 |
| | 3236 | CZ | TYR | 412 | 113.837 | 31.377 | 30.508 | 1.00 | 30.43 |
| | 3237 | OH | TYR | 412 | 113.589 | 30.095 | 30.941 | 1.00 | 25.14 |
| 45 | 3238 | C | TYR | 412 | 115.938 | 37.382 | 28.775 | 1.00 | 18.89 |
| | 3239 | O | TYR | 412 | 116.473 | 37.252 | 27.672 | 1.00 | 21.47 |
| | 3240 | N | LEU | 413 | 115.501 | 38.553 | 29.235 | 1.00 | 22.06 |
| | 3241 | CA | LEU | 413 | 115.620 | 39.790 | 28.460 | 1.00 | 21.99 |
| | 3242 | CB | LEU | 413 | 115.120 | 40.988 | 29.274 | 1.00 | 21.82 |
| 50 | 3243 | CG | LEU | 413 | 113.623 | 40.999 | 29.600 | 1.00 | 28.58 |

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|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 3244 | CD1 | LEU | 413 | 113.286 | 42.192 | 30.481 | 1.00 | 24.87 |
| | 3245 | CD2 | LEU | 413 | 112.806 | 41.026 | 28.316 | 1.00 | 20.55 |
| | 3246 | C | LEU | 413 | 117.008 | 40.081 | 27.901 | 1.00 | 23.58 |
| | 3247 | O | LEU | 413 | 117.157 | 40.329 | 26.702 | 1.00 | 27.31 |
| 5 | 3248 | N | GLY | 414 | 118.018 | 40.041 | 28.764 | 1.00 | 17.88 |
| | 3249 | CA | GLY | 414 | 119.376 | 40.309 | 28.324 | 1.00 | 19.54 |
| | 3250 | C | GLY | 414 | 120.063 | 39.141 | 27.644 | 1.00 | 21.66 |
| | 3251 | O | GLY | 414 | 121.088 | 39.319 | 26.981 | 1.00 | 32.10 |
| | 3252 | N | MET | 415 | 119.500 | 37.947 | 27.804 | 1.00 | 20.71 |
| 10 | 3253 | CA | MET | 415 | 120.062 | 36.741 | 27.209 | 1.00 | 18.08 |
| | 3254 | CB | MET | 415 | 119.440 | 35.504 | 27.850 | 1.00 | 15.67 |
| | 3255 | CG | MET | 415 | 119.705 | 35.424 | 29.345 | 1.00 | 19.68 |
| | 3256 | SD | MET | 415 | 118.883 | 34.052 | 30.144 | 1.00 | 21.56 |
| | 3257 | CE | MET | 415 | 119.945 | 32.725 | 29.700 | 1.00 | 15.56 |
| 15 | 3258 | C | MET | 415 | 119.870 | 36.734 | 25.702 | 1.00 | 23.08 |
| | 3259 | O | MET | 415 | 118.808 | 36.379 | 25.199 | 1.00 | 35.78 |
| | 3260 | N | LYS | 416 | 120.930 | 37.112 | 24.996 | 1.00 | 32.44 |
| | 3261 | CA | LYS | 416 | 120.953 | 37.207 | 23.538 | 1.00 | 38.05 |
| | 3262 | CB | LYS | 416 | 122.360 | 37.608 | 23.090 | 1.00 | 47.08 |
| 20 | 3263 | CG | LYS | 416 | 122.865 | 38.875 | 23.776 | 1.00 | 61.44 |
| | 3264 | CD | LYS | 416 | 124.358 | 39.084 | 23.581 | 1.00 | 67.69 |
| | 3265 | CE | LYS | 416 | 124.846 | 40.273 | 24.399 | 1.00 | 67.49 |
| | 3266 | NZ | LYS | 416 | 126.319 | 40.457 | 24.297 | 1.00 | 75.93 |
| | 3267 | C | LYS | 416 | 120.486 | 35.970 | 22.767 | 1.00 | 39.94 |
| 25 | 3268 | O | LYS | 416 | 120.113 | 36.070 | 21.597 | 1.00 | 44.84 |
| | 3269 | N | SER | 417 | 120.493 | 34.813 | 23.422 | 1.00 | 39.76 |
| | 3270 | CA | SER | 417 | 120.071 | 33.571 | 22.780 | 1.00 | 39.16 |
| | 3271 | CB | SER | 417 | 120.900 | 32.398 | 23.304 | 1.00 | 38.83 |
| | 3272 | OG | SER | 417 | 122.282 | 32.610 | 23.076 | 1.00 | 46.53 |
| 30 | 3273 | C | SER | 417 | 118.581 | 33.270 | 22.956 | 1.00 | 40.99 |
| | 3274 | O | SER | 417 | 118.040 | 32.385 | 22.289 | 1.00 | 41.33 |
| | 3275 | N | ALA | 418 | 117.925 | 34.005 | 23.853 | 1.00 | 38.28 |
| | 3276 | CA | ALA | 418 | 116.501 | 33.814 | 24.122 | 1.00 | 31.24 |
| | 3277 | CB | ALA | 418 | 116.087 | 34.610 | 25.348 | 1.00 | 30.62 |
| 35 | 3278 | C | ALA | 418 | 115.628 | 34.186 | 22.930 | 1.00 | 31.48 |
| | 3279 | O | ALA | 418 | 115.674 | 35.317 | 22.440 | 1.00 | 35.02 |
| | 3280 | N | THR | 419 | 114.841 | 33.219 | 22.468 | 1.00 | 27.95 |
| | 3281 | CA | THR | 419 | 113.942 | 33.409 | 21.332 | 1.00 | 26.20 |
| | 3282 | CB | THR | 419 | 113.996 | 32.197 | 20.370 | 1.00 | 26.76 |
| 40 | 3283 | OG1 | THR | 419 | 113.511 | 31.027 | 21.039 | 1.00 | 27.32 |
| | 3284 | CG2 | THR | 419 | 115.424 | 31.945 | 19.901 | 1.00 | 18.56 |
| | 3285 | C | THR | 419 | 112.502 | 33.595 | 21.806 | 1.00 | 30.31 |
| | 3286 | O | THR | 419 | 112.241 | 33.693 | 23.005 | 1.00 | 33.17 |
| | 3287 | N | GLU | 420 | 111.573 | 33.662 | 20.857 | 1.00 | 35.12 |
| 45 | 3288 | CA | GLU | 420 | 110.158 | 33.818 | 21.183 | 1.00 | 39.51 |
| | 3289 | CB | GLU | 420 | 109.349 | 34.179 | 19.935 | 1.00 | 46.05 |
| | 3290 | CG | GLU | 420 | 108.972 | 35.653 | 19.828 | 1.00 | 51.65 |
| | 3291 | CD | GLU | 420 | 108.013 | 36.104 | 20.919 | 1.00 | 54.36 |
| | 3292 | OE1 | GLU | 420 | 107.027 | 35.384 | 21.192 | 1.00 | 55.36 |
| 50 | 3293 | OE2 | GLU | 420 | 108.245 | 37.186 | 21.500 | 1.00 | 58.01 |

| | | | | | | | | | |
|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 3294 | C | GLU | 420 | 109.620 | 32.527 | 21.781 | 1.00 | 37.05 |
| | 3295 | O | GLU | 420 | 108.852 | 32.550 | 22.742 | 1.00 | 36.79 |
| | 3296 | N | GLN | 421 | 110.050 | 31.404 | 21.215 | 1.00 | 37.04 |
| | 3297 | CA | GLN | 421 | 109.624 | 30.090 | 21.676 | 1.00 | 33.78 |
| 5 | 3298 | CB | GLN | 421 | 110.218 | 28.999 | 20.792 | 1.00 | 40.49 |
| | 3299 | CG | GLN | 421 | 109.711 | 29.009 | 19.363 | 1.00 | 57.72 |
| | 3300 | CD | GLN | 421 | 110.206 | 27.813 | 18.564 | 1.00 | 74.05 |
| | 3301 | OE1 | GLN | 421 | 110.596 | 26.786 | 19.128 | 1.00 | 68.24 |
| | 3302 | NE2 | GLN | 421 | 110.190 | 27.941 | 17.242 | 1.00 | 83.42 |
| 10 | 3303 | C | GLN | 421 | 109.999 | 29.826 | 23.128 | 1.00 | 31.12 |
| | 3304 | O | GLN | 421 | 109.336 | 29.041 | 23.807 | 1.00 | 35.81 |
| | 3305 | N | ASP | 422 | 111.071 | 30.466 | 23.592 | 1.00 | 27.52 |
| | 3306 | CA | ASP | 422 | 111.527 | 30.304 | 24.971 | 1.00 | 25.90 |
| | 3307 | CB | ASP | 422 | 112.963 | 30.821 | 25.137 | 1.00 | 25.75 |
| 15 | 3308 | CG | ASP | 422 | 113.985 | 29.971 | 24.396 | 1.00 | 29.11 |
| | 3309 | OD1 | ASP | 422 | 114.983 | 30.537 | 23.902 | 1.00 | 33.41 |
| | 3310 | OD2 | ASP | 422 | 113.800 | 28.736 | 24.311 | 1.00 | 32.66 |
| | 3311 | C | ASP | 422 | 110.590 | 31.020 | 25.936 | 1.00 | 21.80 |
| | 3312 | O | ASP | 422 | 110.282 | 30.502 | 27.011 | 1.00 | 19.43 |
| 20 | 3313 | N | PHE | 423 | 110.145 | 32.213 | 25.545 | 1.00 | 24.75 |
| | 3314 | CA | PHE | 423 | 109.223 | 33.004 | 26.357 | 1.00 | 26.23 |
| | 3315 | CB | PHE | 423 | 109.117 | 34.432 | 25.818 | 1.00 | 30.85 |
| | 3316 | CG | PHE | 423 | 110.290 | 35.306 | 26.166 | 1.00 | 32.84 |
| | 3317 | CD1 | PHE | 423 | 111.336 | 35.482 | 25.268 | 1.00 | 34.61 |
| 25 | 3318 | CD2 | PHE | 423 | 110.338 | 35.972 | 27.388 | 1.00 | 33.51 |
| | 3319 | CE1 | PHE | 423 | 112.412 | 36.312 | 25.579 | 1.00 | 30.52 |
| | 3320 | CE2 | PHE | 423 | 111.410 | 36.805 | 27.708 | 1.00 | 35.27 |
| | 3321 | CZ | PHE | 423 | 112.448 | 36.974 | 26.801 | 1.00 | 23.59 |
| | 3322 | C | PHE | 423 | 107.849 | 32.354 | 26.330 | 1.00 | 24.84 |
| 30 | 3323 | O | PHE | 423 | 107.106 | 32.392 | 27.311 | 1.00 | 31.10 |
| | 3324 | N | GLU | 424 | 107.530 | 31.751 | 25.191 | 1.00 | 29.70 |
| | 3325 | CA | GLU | 424 | 106.261 | 31.070 | 24.982 | 1.00 | 36.07 |
| | 3326 | CB | GLU | 424 | 106.187 | 30.588 | 23.535 | 1.00 | 40.70 |
| | 3327 | CG | GLU | 424 | 104.785 | 30.391 | 22.992 | 1.00 | 63.10 |
| 35 | 3328 | CD | GLU | 424 | 104.759 | 30.296 | 21.473 | 1.00 | 75.17 |
| | 3329 | OE1 | GLU | 424 | 105.781 | 29.898 | 20.867 | 1.00 | 75.10 |
| | 3330 | OE2 | GLU | 424 | 103.710 | 30.630 | 20.880 | 1.00 | 85.30 |
| | 3331 | C | GLU | 424 | 106.164 | 29.892 | 25.949 | 1.00 | 31.83 |
| | 3332 | O | GLU | 424 | 105.138 | 29.687 | 26.595 | 1.00 | 35.87 |
| 40 | 3333 | N | TRP | 425 | 107.258 | 29.148 | 26.066 | 1.00 | 29.46 |
| | 3334 | CA | TRP | 425 | 107.339 | 27.999 | 26.958 | 1.00 | 23.86 |
| | 3335 | CB | TRP | 425 | 108.680 | 27.285 | 26.753 | 1.00 | 25.55 |
| | 3336 | CG | TRP | 425 | 108.991 | 26.265 | 27.803 | 1.00 | 29.41 |
| | 3337 | CD2 | TRP | 425 | 109.808 | 26.455 | 28.965 | 1.00 | 27.61 |
| 45 | 3338 | CE2 | TRP | 425 | 109.779 | 25.249 | 29.697 | 1.00 | 24.31 |
| | 3339 | CE3 | TRP | 425 | 110.557 | 27.529 | 29.460 | 1.00 | 30.25 |
| | 3340 | CD1 | TRP | 425 | 108.521 | 24.984 | 27.871 | 1.00 | 28.89 |
| | 3341 | NE1 | TRP | 425 | 108.987 | 24.369 | 29.007 | 1.00 | 29.83 |
| | 3342 | CZ2 | TRP | 425 | 110.473 | 25.087 | 30.900 | 1.00 | 16.37 |
| 50 | 3343 | CZ3 | TRP | 425 | 111.245 | 27.367 | 30.658 | 1.00 | 25.72 |

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|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 3344 | CH2 | TRP | 425 | 111.196 | 26.154 | 31.363 | 1.00 | 19.53 |
| | 3345 | C | TRP | 425 | 107.205 | 28.437 | 28.414 | 1.00 | 25.64 |
| | 3346 | O | TRP | 425 | 106.523 | 27.792 | 29.213 | 1.00 | 26.99 |
| 5 | 3347 | N | LEU | 426 | 107.852 | 29.553 | 28.739 | 1.00 | 26.42 |
| | 3348 | CA | LEU | 426 | 107.853 | 30.103 | 30.088 | 1.00 | 21.18 |
| | 3349 | CB | LEU | 426 | 108.922 | 31.191 | 30.195 | 1.00 | 21.43 |
| | 3350 | CG | LEU | 426 | 109.379 | 31.600 | 31.595 | 1.00 | 14.19 |
| | 3351 | CD1 | LEU | 426 | 110.106 | 30.441 | 32.251 | 1.00 | 14.14 |
| 10 | 3352 | CD2 | LEU | 426 | 110.297 | 32.798 | 31.499 | 1.00 | 12.82 |
| | 3353 | C | LEU | 426 | 106.504 | 30.664 | 30.523 | 1.00 | 23.80 |
| | 3354 | O | LEU | 426 | 106.153 | 30.596 | 31.702 | 1.00 | 31.77 |
| | 3355 | N | SER | 427 | 105.754 | 31.221 | 29.575 | 1.00 | 28.08 |
| | 3356 | CA | SER | 427 | 104.444 | 31.802 | 29.871 | 1.00 | 30.28 |
| | 3357 | CB | SER | 427 | 103.915 | 32.592 | 28.665 | 1.00 | 26.14 |
| 15 | 3358 | OG | SER | 427 | 103.742 | 31.763 | 27.528 | 1.00 | 29.08 |
| | 3359 | C | SER | 427 | 103.406 | 30.773 | 30.325 | 1.00 | 29.36 |
| | 3360 | O | SER | 427 | 102.497 | 31.099 | 31.088 | 1.00 | 31.12 |
| | 3361 | N | LYS | 428 | 103.558 | 29.530 | 29.873 | 1.00 | 27.92 |
| 20 | 3362 | CA | LYS | 428 | 102.637 | 28.455 | 30.230 | 1.00 | 20.58 |
| | 3363 | CB | LYS | 428 | 102.770 | 27.290 | 29.251 | 1.00 | 23.24 |
| | 3364 | CG | LYS | 428 | 102.454 | 27.613 | 27.801 | 1.00 | 22.85 |
| | 3365 | CD | LYS | 428 | 102.509 | 26.335 | 26.976 | 1.00 | 42.29 |
| | 3366 | CE | LYS | 428 | 102.338 | 26.597 | 25.493 | 1.00 | 49.89 |
| | 3367 | NZ | LYS | 428 | 102.345 | 25.316 | 24.727 | 1.00 | 62.04 |
| 25 | 3368 | C | LYS | 428 | 102.844 | 27.935 | 31.654 | 1.00 | 20.72 |
| | 3369 | O | LYS | 428 | 102.183 | 26.980 | 32.067 | 1.00 | 29.09 |
| | 3370 | N | ASN | 429 | 103.762 | 28.557 | 32.391 | 1.00 | 20.35 |
| | 3371 | CA | ASN | 429 | 104.072 | 28.170 | 33.770 | 1.00 | 14.44 |
| | 3372 | CB | ASN | 429 | 102.868 | 28.406 | 34.685 | 1.00 | 13.93 |
| 30 | 3373 | CG | ASN | 429 | 102.581 | 29.876 | 34.910 | 1.00 | 21.29 |
| | 3374 | OD1 | ASN | 429 | 103.306 | 30.747 | 34.431 | 1.00 | 26.38 |
| | 3375 | ND2 | ASN | 429 | 101.522 | 30.159 | 35.657 | 1.00 | 28.12 |
| | 3376 | C | ASN | 429 | 104.545 | 26.724 | 33.900 | 1.00 | 19.87 |
| | 3377 | O | ASN | 429 | 103.831 | 25.868 | 34.426 | 1.00 | 27.89 |
| 35 | 3378 | N | PRO | 430 | 105.764 | 26.433 | 33.418 | 1.00 | 18.35 |
| | 3379 | CD | PRO | 430 | 106.650 | 27.362 | 32.701 | 1.00 | 19.00 |
| | 3380 | CA | PRO | 430 | 106.358 | 25.096 | 33.468 | 1.00 | 11.22 |
| | 3381 | CB | PRO | 430 | 107.711 | 25.309 | 32.808 | 1.00 | 15.49 |
| | 3382 | CG | PRO | 430 | 107.444 | 26.425 | 31.859 | 1.00 | 26.05 |
| 40 | 3383 | C | PRO | 430 | 106.518 | 24.612 | 34.902 | 1.00 | 17.61 |
| | 3384 | O | PRO | 430 | 106.617 | 25.416 | 35.828 | 1.00 | 19.92 |
| | 3385 | N | LYS | 431 | 106.569 | 23.294 | 35.073 | 1.00 | 18.71 |
| | 3386 | CA | LYS | 431 | 106.699 | 22.681 | 36.389 | 1.00 | 14.83 |
| | 3387 | CB | LYS | 431 | 106.682 | 21.157 | 36.256 | 1.00 | 15.08 |
| 45 | 3388 | CG | LYS | 431 | 106.353 | 20.409 | 37.539 | 1.00 | 26.85 |
| | 3389 | CD | LYS | 431 | 106.103 | 18.937 | 37.244 | 1.00 | 41.27 |
| | 3390 | CE | LYS | 431 | 105.561 | 18.195 | 38.455 | 1.00 | 49.80 |
| | 3391 | NZ | LYS | 431 | 105.297 | 16.760 | 38.140 | 1.00 | 45.04 |
| | 3392 | C | LYS | 431 | 107.959 | 23.137 | 37.121 | 1.00 | 19.80 |
| 50 | 3393 | O | LYS | 431 | 107.937 | 23.333 | 38.338 | 1.00 | 20.81 |

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|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 3394 | N | ILE | 432 | 109.051 | 23.316 | 36.380 | 1.00 | 15.93 |
| | 3395 | CA | ILE | 432 | 110.306 | 23.757 | 36.979 | 1.00 | 16.86 |
| | 3396 | CB | ILE | 432 | 111.497 | 23.632 | 35.994 | 1.00 | 20.40 |
| | 3397 | CG2 | ILE | 432 | 111.278 | 24.502 | 34.756 | 1.00 | 16.63 |
| 5 | 3398 | CG1 | ILE | 432 | 112.804 | 23.985 | 36.709 | 1.00 | 14.19 |
| | 3399 | CD1 | ILE | 432 | 114.048 | 23.649 | 35.920 | 1.00 | 13.37 |
| | 3400 | C | ILE | 432 | 110.182 | 25.187 | 37.499 | 1.00 | 17.42 |
| | 3401 | O | ILE | 432 | 110.681 | 25.508 | 38.579 | 1.00 | 24.54 |
| | 3402 | N | LEU | 433 | 109.488 | 26.035 | 36.742 | 1.00 | 15.09 |
| 10 | 3403 | CA | LEU | 433 | 109.277 | 27.420 | 37.146 | 1.00 | 14.83 |
| | 3404 | CB | LEU | 433 | 108.728 | 28.245 | 35.978 | 1.00 | 13.49 |
| | 3405 | CG | LEU | 433 | 108.378 | 29.708 | 36.272 | 1.00 | 10.45 |
| | 3406 | CD1 | LEU | 433 | 109.564 | 30.430 | 36.896 | 1.00 | 15.23 |
| | 3407 | CD2 | LEU | 433 | 107.939 | 30.400 | 34.993 | 1.00 | 9.30 |
| 15 | 3408 | C | LEU | 433 | 108.289 | 27.433 | 38.304 | 1.00 | 18.07 |
| | 3409 | O | LEU | 433 | 108.481 | 28.140 | 39.295 | 1.00 | 21.14 |
| | 3410 | N | GLU | 434 | 107.245 | 26.621 | 38.173 | 1.00 | 21.38 |
| | 3411 | CA | GLU | 434 | 106.209 | 26.503 | 39.188 | 1.00 | 16.25 |
| | 3412 | CB | GLU | 434 | 105.184 | 25.452 | 38.753 | 1.00 | 23.52 |
| 20 | 3413 | CG | GLU | 434 | 103.812 | 25.605 | 39.385 | 1.00 | 38.66 |
| | 3414 | CD | GLU | 434 | 103.161 | 26.933 | 39.037 | 1.00 | 42.62 |
| | 3415 | OE1 | GLU | 434 | 102.828 | 27.148 | 37.851 | 1.00 | 32.73 |
| | 3416 | OE2 | GLU | 434 | 102.993 | 27.765 | 39.953 | 1.00 | 37.72 |
| | 3417 | C | GLU | 434 | 106.850 | 26.095 | 40.511 | 1.00 | 14.12 |
| 25 | 3418 | O | GLU | 434 | 106.561 | 26.676 | 41.556 | 1.00 | 14.76 |
| | 3419 | N | ALA | 435 | 107.753 | 25.120 | 40.440 | 1.00 | 17.75 |
| | 3420 | CA | ALA | 435 | 108.465 | 24.610 | 41.610 | 1.00 | 16.67 |
| | 3421 | CB | ALA | 435 | 109.303 | 23.410 | 41.214 | 1.00 | 8.83 |
| | 3422 | C | ALA | 435 | 109.344 | 25.683 | 42.254 | 1.00 | 11.99 |
| 30 | 3423 | O | ALA | 435 | 109.372 | 25.827 | 43.477 | 1.00 | 7.99 |
| | 3424 | N | SER | 436 | 110.057 | 26.435 | 41.422 | 1.00 | 15.97 |
| | 3425 | CA | SER | 436 | 110.924 | 27.508 | 41.900 | 1.00 | 21.95 |
| | 3426 | CB | SER | 436 | 111.636 | 28.163 | 40.713 | 1.00 | 24.20 |
| | 3427 | OG | SER | 436 | 112.489 | 29.212 | 41.135 | 1.00 | 40.93 |
| 35 | 3428 | C | SER | 436 | 110.110 | 28.554 | 42.674 | 1.00 | 21.39 |
| | 3429 | O | SER | 436 | 110.519 | 29.009 | 43.748 | 1.00 | 24.40 |
| | 3430 | N | VAL | 437 | 108.951 | 28.912 | 42.125 | 1.00 | 18.68 |
| | 3431 | CA | VAL | 437 | 108.054 | 29.889 | 42.739 | 1.00 | 8.95 |
| | 3432 | CB | VAL | 437 | 106.855 | 30.188 | 41.818 | 1.00 | 11.54 |
| 40 | 3433 | CG1 | VAL | 437 | 105.917 | 31.169 | 42.478 | 1.00 | 11.34 |
| | 3434 | CG2 | VAL | 437 | 107.339 | 30.734 | 40.486 | 1.00 | 5.44 |
| | 3435 | C | VAL | 437 | 107.533 | 29.401 | 44.092 | 1.00 | 9.21 |
| | 3436 | O | VAL | 437 | 107.452 | 30.176 | 45.048 | 1.00 | 12.18 |
| | 3437 | N | ILE | 438 | 107.185 | 28.115 | 44.161 | 1.00 | 9.76 |
| 45 | 3438 | CA | ILE | 438 | 106.673 | 27.504 | 45.388 | 1.00 | 8.03 |
| | 3439 | CB | ILE | 438 | 106.309 | 26.015 | 45.171 | 1.00 | 14.49 |
| | 3440 | CG2 | ILE | 438 | 105.931 | 25.360 | 46.500 | 1.00 | 10.62 |
| | 3441 | CG1 | ILE | 438 | 105.162 | 25.896 | 44.164 | 1.00 | 23.13 |
| | 3442 | CD1 | ILE | 438 | 104.753 | 24.468 | 43.853 | 1.00 | 31.20 |
| 50 | 3443 | C | ILE | 438 | 107.692 | 27.603 | 46.520 | 1.00 | 12.21 |

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|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 3444 | O | ILE | 438 | 107.349 | 27.982 | 47.639 | 1.00 | 18.63 |
| | 3445 | N | ILE | 439 | 108.941 | 27.258 | 46.216 | 1.00 | 14.08 |
| | 3446 | CA | ILE | 439 | 110.033 | 27.307 | 47.188 | 1.00 | 9.89 |
| | 3447 | CB | ILE | 439 | 111.369 | 26.901 | 46.525 | 1.00 | 12.54 |
| 5 | 3448 | CG2 | ILE | 439 | 112.540 | 27.161 | 47.459 | 1.00 | 11.31 |
| | 3449 | CG1 | ILE | 439 | 111.321 | 25.424 | 46.136 | 1.00 | 2.00 |
| | 3450 | CD1 | ILE | 439 | 112.441 | 24.990 | 45.233 | 1.00 | 14.05 |
| | 3451 | C | ILE | 439 | 110.152 | 28.706 | 47.783 | 1.00 | 9.52 |
| | 3452 | O | ILE | 439 | 110.213 | 28.871 | 49.003 | 1.00 | 10.13 |
| 10 | 3453 | N | CYS | 440 | 110.135 | 29.714 | 46.918 | 1.00 | 8.13 |
| | 3454 | CA | CYS | 440 | 110.233 | 31.098 | 47.361 | 1.00 | 12.62 |
| | 3455 | CB | CYS | 440 | 110.267 | 32.036 | 46.153 | 1.00 | 5.84 |
| | 3456 | SG | CYS | 440 | 110.449 | 33.774 | 46.599 | 1.00 | 11.97 |
| | 3457 | C | CYS | 440 | 109.073 | 31.482 | 48.283 | 1.00 | 17.47 |
| 15 | 3458 | O | CYS | 440 | 109.264 | 32.175 | 49.287 | 1.00 | 18.40 |
| | 3459 | N | ARG | 441 | 107.875 | 31.012 | 47.940 | 1.00 | 18.94 |
| | 3460 | CA | ARG | 441 | 106.669 | 31.296 | 48.714 | 1.00 | 11.76 |
| | 3461 | CB | ARG | 441 | 105.433 | 30.810 | 47.949 | 1.00 | 10.60 |
| | 3462 | CG | ARG | 441 | 104.093 | 31.083 | 48.629 | 1.00 | 6.45 |
| 20 | 3463 | CD | ARG | 441 | 103.718 | 32.559 | 48.590 | 1.00 | 19.08 |
| | 3464 | NE | ARG | 441 | 104.454 | 33.353 | 49.571 | 1.00 | 23.16 |
| | 3465 | CZ | ARG | 441 | 104.623 | 34.670 | 49.500 | 1.00 | 20.47 |
| | 3466 | NH1 | ARG | 441 | 104.108 | 35.353 | 48.489 | 1.00 | 12.16 |
| | 3467 | NH2 | ARG | 441 | 105.307 | 35.307 | 50.441 | 1.00 | 30.69 |
| 25 | 3468 | C | ARG | 441 | 106.716 | 30.637 | 50.089 | 1.00 | 17.00 |
| | 3469 | O | ARG | 441 | 106.629 | 31.307 | 51.120 | 1.00 | 25.77 |
| | 3470 | N | VAL | 442 | 106.858 | 29.317 | 50.086 | 1.00 | 22.16 |
| | 3471 | CA | VAL | 442 | 106.920 | 28.518 | 51.306 | 1.00 | 22.25 |
| | 3472 | CB | VAL | 442 | 107.112 | 27.032 | 50.959 | 1.00 | 23.82 |
| 30 | 3473 | CG1 | VAL | 442 | 107.624 | 26.261 | 52.164 | 1.00 | 26.50 |
| | 3474 | CG2 | VAL | 442 | 105.796 | 26.450 | 50.471 | 1.00 | 31.37 |
| | 3475 | C | VAL | 442 | 108.004 | 28.969 | 52.283 | 1.00 | 21.17 |
| | 3476 | O | VAL | 442 | 107.765 | 29.058 | 53.488 | 1.00 | 25.05 |
| | 3477 | N | ILE | 443 | 109.195 | 29.243 | 51.761 | 1.00 | 22.99 |
| 35 | 3478 | CA | ILE | 443 | 110.305 | 29.685 | 52.596 | 1.00 | 27.94 |
| | 3479 | CB | ILE | 443 | 111.628 | 29.710 | 51.805 | 1.00 | 34.71 |
| | 3480 | CG2 | ILE | 443 | 112.721 | 30.396 | 52.612 | 1.00 | 32.63 |
| | 3481 | CG1 | ILE | 443 | 112.041 | 28.279 | 51.458 | 1.00 | 35.15 |
| | 3482 | CD1 | ILE | 443 | 113.322 | 28.183 | 50.669 | 1.00 | 41.45 |
| 40 | 3483 | C | ILE | 443 | 110.024 | 31.054 | 53.208 | 1.00 | 24.50 |
| | 3484 | O | ILE | 443 | 110.253 | 31.263 | 54.400 | 1.00 | 25.69 |
| | 3485 | N | ASP | 444 | 109.500 | 31.972 | 52.398 | 1.00 | 24.21 |
| | 3486 | CA | ASP | 444 | 109.178 | 33.314 | 52.875 | 1.00 | 26.25 |
| | 3487 | CB | ASP | 444 | 108.695 | 34.203 | 51.721 | 1.00 | 29.76 |
| 45 | 3488 | CG | ASP | 444 | 108.365 | 35.624 | 52.169 | 1.00 | 39.45 |
| | 3489 | OD1 | ASP | 444 | 109.179 | 36.535 | 51.910 | 1.00 | 45.87 |
| | 3490 | OD2 | ASP | 444 | 107.288 | 35.841 | 52.768 | 1.00 | 45.57 |
| | 3491 | C | ASP | 444 | 108.103 | 33.247 | 53.952 | 1.00 | 28.37 |
| | 3492 | O | ASP | 444 | 108.228 | 33.883 | 54.995 | 1.00 | 29.64 |
| 50 | 3493 | N | ASP | 445 | 107.061 | 32.458 | 53.700 | 1.00 | 30.42 |

| | | | | | | | | | |
|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 3494 | CA | ASP | 445 | 105.950 | 32.318 | 54.637 | 1.00 | 32.30 |
| | 3495 | CB | ASP | 445 | 104.797 | 31.544 | 53.994 | 1.00 | 33.98 |
| | 3496 | CG | ASP | 445 | 104.151 | 32.302 | 52.838 | 1.00 | 37.92 |
| | 3497 | OD1 | ASP | 445 | 104.356 | 33.532 | 52.717 | 1.00 | 38.86 |
| 5 | 3498 | OD2 | ASP | 445 | 103.429 | 31.662 | 52.047 | 1.00 | 28.07 |
| | 3499 | C | ASP | 445 | 106.335 | 31.690 | 55.970 | 1.00 | 33.30 |
| | 3500 | O | ASP | 445 | 105.762 | 32.030 | 57.009 | 1.00 | 42.91 |
| | 3501 | N | THR | 446 | 107.302 | 30.778 | 55.946 | 1.00 | 33.28 |
| | 3502 | CA | THR | 446 | 107.758 | 30.124 | 57.168 | 1.00 | 30.88 |
| 10 | 3503 | CB | THR | 446 | 108.625 | 28.887 | 56.855 | 1.00 | 26.02 |
| | 3504 | OG1 | THR | 446 | 107.873 | 27.969 | 56.050 | 1.00 | 21.99 |
| | 3505 | CG2 | THR | 446 | 109.046 | 28.188 | 58.143 | 1.00 | 25.74 |
| | 3506 | C | THR | 446 | 108.570 | 31.110 | 58.014 | 1.00 | 32.83 |
| | 3507 | O | THR | 446 | 108.459 | 31.131 | 59.238 | 1.00 | 33.61 |
| 15 | 3508 | N | ALA | 447 | 109.357 | 31.944 | 57.339 | 1.00 | 40.56 |
| | 3509 | CA | ALA | 447 | 110.202 | 32.937 | 57.996 | 1.00 | 45.46 |
| | 3510 | CB | ALA | 447 | 111.313 | 33.374 | 57.056 | 1.00 | 42.21 |
| | 3511 | C | ALA | 447 | 109.434 | 34.155 | 58.468 | 1.00 | 46.97 |
| | 3512 | O | ALA | 447 | 109.596 | 34.617 | 59.599 | 1.00 | 54.11 |
| 20 | 3513 | N | THR | 448 | 108.599 | 34.690 | 57.581 | 1.00 | 47.28 |
| | 3514 | CA | THR | 448 | 107.832 | 35.884 | 57.879 | 1.00 | 46.44 |
| | 3515 | CB | THR | 448 | 107.689 | 36.787 | 56.618 | 1.00 | 41.12 |
| | 3516 | OG1 | THR | 448 | 106.943 | 36.112 | 55.607 | 1.00 | 30.26 |
| | 3517 | CG2 | THR | 448 | 109.064 | 37.170 | 56.071 | 1.00 | 32.60 |
| 25 | 3518 | C | THR | 448 | 106.446 | 35.694 | 58.497 | 1.00 | 51.30 |
| | 3519 | O | THR | 448 | 105.708 | 36.657 | 58.620 | 1.00 | 53.69 |
| | 3520 | N | TYR | 449 | 106.080 | 34.481 | 58.912 | 1.00 | 53.28 |
| | 3521 | CA | TYR | 449 | 104.751 | 34.282 | 59.492 | 1.00 | 58.27 |
| | 3522 | CB | TYR | 449 | 104.497 | 32.811 | 59.888 | 1.00 | 58.98 |
| 30 | 3523 | CG | TYR | 449 | 103.175 | 32.661 | 60.637 | 1.00 | 61.56 |
| | 3524 | CD1 | TYR | 449 | 101.973 | 33.066 | 60.055 | 1.00 | 66.72 |
| | 3525 | CE1 | TYR | 449 | 100.772 | 33.026 | 60.769 | 1.00 | 64.98 |
| | 3526 | CD2 | TYR | 449 | 103.147 | 32.198 | 61.957 | 1.00 | 62.94 |
| | 3527 | CE2 | TYR | 449 | 101.956 | 32.155 | 62.672 | 1.00 | 66.76 |
| 35 | 3528 | CZ | TYR | 449 | 100.773 | 32.575 | 62.080 | 1.00 | 67.45 |
| | 3529 | OH | TYR | 449 | 99.601 | 32.590 | 62.810 | 1.00 | 73.04 |
| | 3530 | C | TYR | 449 | 104.462 | 35.189 | 60.691 | 1.00 | 59.96 |
| | 3531 | O | TYR | 449 | 103.576 | 36.051 | 60.638 | 1.00 | 60.11 |
| | 3532 | N | GLU | 450 | 105.199 | 34.975 | 61.771 | 1.00 | 61.73 |
| 40 | 3533 | CA | GLU | 450 | 105.029 | 35.733 | 62.995 | 1.00 | 61.61 |
| | 3534 | CB | GLU | 450 | 106.071 | 35.308 | 64.025 | 1.00 | 65.21 |
| | 3535 | CG | GLU | 450 | 105.833 | 33.912 | 64.589 | 1.00 | 75.41 |
| | 3536 | CD | GLU | 450 | 106.887 | 33.502 | 65.610 | 1.00 | 85.43 |
| | 3537 | OE1 | GLU | 450 | 107.416 | 34.375 | 66.331 | 1.00 | 91.32 |
| 45 | 3538 | OE2 | GLU | 450 | 107.196 | 32.293 | 65.686 | 1.00 | 90.42 |
| | 3539 | C | GLU | 450 | 105.026 | 37.251 | 62.841 | 1.00 | 59.86 |
| | 3540 | O | GLU | 450 | 104.144 | 37.918 | 63.377 | 1.00 | 59.89 |
| | 3541 | N | VAL | 451 | 105.995 | 37.787 | 62.098 | 1.00 | 61.44 |
| | 3542 | CA | VAL | 451 | 106.092 | 39.234 | 61.873 | 1.00 | 63.11 |
| 50 | 3543 | CB | VAL | 451 | 107.408 | 39.596 | 61.116 | 1.00 | 64.01 |

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|----|------|-----|-----|-----|---------|--------|--------|------|--------|
| | 3544 | CG1 | VAL | 451 | 107.256 | 40.886 | 60.304 | 1.00 | 63.92 |
| | 3545 | CG2 | VAL | 451 | 108.541 | 39.761 | 62.123 | 1.00 | 71.39 |
| | 3546 | C | VAL | 451 | 104.881 | 39.809 | 61.152 | 1.00 | 62.77 |
| 5 | 3547 | O | VAL | 451 | 104.336 | 40.841 | 61.555 | 1.00 | 65.95 |
| | 3548 | N | GLU | 452 | 104.450 | 39.118 | 60.103 | 1.00 | 62.77 |
| | 3549 | CA | GLU | 452 | 103.304 | 39.545 | 59.315 | 1.00 | 57.61 |
| | 3550 | CB | GLU | 452 | 103.275 | 38.782 | 57.991 | 1.00 | 56.30 |
| | 3551 | CG | GLU | 452 | 104.444 | 39.130 | 57.058 | 1.00 | 59.48 |
| 10 | 3552 | CD | GLU | 452 | 104.469 | 38.317 | 55.787 | 1.00 | 60.10 |
| | 3553 | OE1 | GLU | 452 | 104.787 | 38.899 | 54.728 | 1.00 | 62.60 |
| | 3554 | OE2 | GLU | 452 | 104.183 | 37.106 | 55.843 | 1.00 | 61.28 |
| | 3555 | C | GLU | 452 | 101.984 | 39.392 | 60.081 | 1.00 | 56.17 |
| | 3556 | O | GLU | 452 | 101.034 | 40.136 | 59.838 | 1.00 | 51.59 |
| 15 | 3557 | N | LYS | 453 | 101.946 | 38.466 | 61.040 | 1.00 | 58.80 |
| | 3558 | CA | LYS | 453 | 100.753 | 38.241 | 61.858 | 1.00 | 58.04 |
| | 3559 | CB | LYS | 453 | 100.863 | 36.913 | 62.611 | 1.00 | 59.76 |
| | 3560 | CG | LYS | 453 | 99.644 | 36.565 | 63.453 | 1.00 | 60.02 |
| | 3561 | CD | LYS | 453 | 99.925 | 35.384 | 64.366 | 1.00 | 58.67 |
| 20 | 3562 | CE | LYS | 453 | 98.732 | 35.093 | 65.262 | 1.00 | 61.72 |
| | 3563 | NZ | LYS | 453 | 99.013 | 33.991 | 66.222 | 1.00 | 58.55 |
| | 3564 | C | LYS | 453 | 100.584 | 39.385 | 62.863 | 1.00 | 57.99 |
| | 3565 | O | LYS | 453 | 99.461 | 39.769 | 63.195 | 1.00 | 57.81 |
| | 3566 | N | SER | 454 | 101.709 | 39.920 | 63.339 | 1.00 | 62.23 |
| 25 | 3567 | CA | SER | 454 | 101.712 | 41.026 | 64.295 | 1.00 | 61.09 |
| | 3568 | CB | SER | 454 | 103.125 | 41.265 | 64.837 | 1.00 | 60.66 |
| | 3569 | OG | SER | 454 | 103.548 | 40.191 | 65.654 | 1.00 | 66.36 |
| | 3570 | C | SER | 454 | 101.185 | 42.311 | 63.665 | 1.00 | 58.28 |
| | 3571 | O | SER | 454 | 100.632 | 43.163 | 64.360 | 1.00 | 56.27 |
| 30 | 3572 | N | ARG | 455 | 101.373 | 42.447 | 62.354 | 1.00 | 58.50 |
| | 3573 | CA | ARG | 455 | 100.916 | 43.623 | 61.619 | 1.00 | 62.35 |
| | 3574 | CB | ARG | 455 | 101.827 | 43.885 | 60.414 | 1.00 | 67.55 |
| | 3575 | CG | ARG | 455 | 103.261 | 44.228 | 60.797 | 1.00 | 76.19 |
| | 3576 | CD | ARG | 455 | 104.115 | 44.547 | 59.581 | 1.00 | 85.72 |
| 35 | 3577 | NE | ARG | 455 | 105.444 | 45.024 | 59.964 | 1.00 | 96.37 |
| | 3578 | CZ | ARG | 455 | 106.292 | 45.634 | 59.140 | 1.00 | 100.00 |
| | 3579 | NH1 | ARG | 455 | 105.960 | 45.845 | 57.872 | 1.00 | 100.00 |
| | 3580 | NH2 | ARG | 455 | 107.470 | 46.051 | 59.587 | 1.00 | 99.29 |
| | 3581 | C | ARG | 455 | 99.457 | 43.503 | 61.176 | 1.00 | 60.13 |
| 40 | 3582 | O | ARG | 455 | 98.922 | 44.399 | 60.519 | 1.00 | 58.35 |
| | 3583 | N | GLY | 456 | 98.824 | 42.391 | 61.546 | 1.00 | 60.37 |
| | 3584 | CA | GLY | 456 | 97.432 | 42.164 | 61.201 | 1.00 | 62.20 |
| | 3585 | C | GLY | 456 | 97.183 | 41.378 | 59.925 | 1.00 | 67.18 |
| | 3586 | O | GLY | 456 | 96.036 | 41.048 | 59.626 | 1.00 | 70.98 |
| 45 | 3587 | N | GLN | 457 | 98.238 | 41.091 | 59.166 | 1.00 | 69.31 |
| | 3588 | CA | GLN | 457 | 98.108 | 40.340 | 57.917 | 1.00 | 68.54 |
| | 3589 | CB | GLN | 457 | 99.397 | 40.438 | 57.089 | 1.00 | 69.51 |
| | 3590 | CG | GLN | 457 | 99.764 | 41.859 | 56.671 | 1.00 | 74.48 |
| | 3591 | CD | GLN | 457 | 101.105 | 41.941 | 55.965 | 1.00 | 78.04 |
| 50 | 3592 | OE1 | GLN | 457 | 102.099 | 41.389 | 56.428 | 1.00 | 87.45 |
| | 3593 | NE2 | GLN | 457 | 101.140 | 42.651 | 54.840 | 1.00 | 80.41 |

| | | | | | | | | | |
|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 3594 | C | GLN | 457 | 97.765 | 38.879 | 58.197 | 1.00 | 66.56 |
| | 3595 | O | GLN | 457 | 98.645 | 38.020 | 58.262 | 1.00 | 70.53 |
| | 3596 | N | ILE | 458 | 96.475 | 38.616 | 58.384 | 1.00 | 64.43 |
| 5 | 3597 | CA | ILE | 458 | 95.976 | 37.272 | 58.664 | 1.00 | 60.84 |
| | 3598 | CB | ILE | 458 | 94.652 | 37.317 | 59.458 | 1.00 | 62.21 |
| | 3599 | CG2 | ILE | 458 | 94.940 | 37.397 | 60.958 | 1.00 | 64.20 |
| | 3600 | CG1 | ILE | 458 | 93.769 | 38.462 | 58.943 | 1.00 | 60.42 |
| | 3601 | CD1 | ILE | 458 | 92.437 | 38.608 | 59.656 | 1.00 | 66.77 |
| 10 | 3602 | C | ILE | 458 | 95.768 | 36.440 | 57.403 | 1.00 | 55.84 |
| | 3603 | O | ILE | 458 | 95.281 | 35.310 | 57.468 | 1.00 | 51.58 |
| | 3604 | N | ALA | 459 | 96.145 | 37.005 | 56.259 | 1.00 | 58.27 |
| | 3605 | CA | ALA | 459 | 96.011 | 36.318 | 54.979 | 1.00 | 56.90 |
| | 3606 | CB | ALA | 459 | 95.609 | 37.305 | 53.888 | 1.00 | 56.20 |
| 15 | 3607 | C | ALA | 459 | 97.296 | 35.587 | 54.579 | 1.00 | 54.74 |
| | 3608 | O | ALA | 459 | 97.434 | 35.158 | 53.433 | 1.00 | 54.48 |
| | 3609 | N | THR | 460 | 98.236 | 35.455 | 55.513 | 1.00 | 49.39 |
| | 3610 | CA | THR | 460 | 99.494 | 34.779 | 55.224 | 1.00 | 47.02 |
| | 3611 | CB | THR | 460 | 100.603 | 35.180 | 56.200 | 1.00 | 50.43 |
| 20 | 3612 | OG1 | THR | 460 | 100.077 | 35.259 | 57.532 | 1.00 | 52.34 |
| | 3613 | CG2 | THR | 460 | 101.194 | 36.507 | 55.781 | 1.00 | 56.05 |
| | 3614 | C | THR | 460 | 99.399 | 33.264 | 55.164 | 1.00 | 45.28 |
| | 3615 | O | THR | 460 | 98.566 | 32.651 | 55.832 | 1.00 | 47.09 |
| | 3616 | N | GLY | 461 | 100.303 | 32.676 | 54.386 | 1.00 | 45.02 |
| 25 | 3617 | CA | GLY | 461 | 100.351 | 31.238 | 54.190 | 1.00 | 41.47 |
| | 3618 | C | GLY | 461 | 100.107 | 30.318 | 55.367 | 1.00 | 38.12 |
| | 3619 | O | GLY | 461 | 99.172 | 29.516 | 55.341 | 1.00 | 41.90 |
| | 3620 | N | ILE | 462 | 100.962 | 30.399 | 56.380 | 1.00 | 36.28 |
| | 3621 | CA | ILE | 462 | 100.825 | 29.545 | 57.552 | 1.00 | 41.08 |
| 30 | 3622 | CB | ILE | 462 | 101.954 | 29.813 | 58.580 | 1.00 | 34.80 |
| | 3623 | CG2 | ILE | 462 | 101.814 | 28.893 | 59.792 | 1.00 | 33.01 |
| | 3624 | CG1 | ILE | 462 | 103.319 | 29.613 | 57.917 | 1.00 | 21.22 |
| | 3625 | CD1 | ILE | 462 | 103.525 | 28.231 | 57.322 | 1.00 | 17.74 |
| | 3626 | C | ILE | 462 | 99.444 | 29.683 | 58.197 | 1.00 | 47.74 |
| 35 | 3627 | O | ILE | 462 | 98.823 | 28.682 | 58.556 | 1.00 | 53.27 |
| | 3628 | N | GLU | 463 | 98.940 | 30.915 | 58.266 | 1.00 | 49.04 |
| | 3629 | CA | GLU | 463 | 97.626 | 31.178 | 58.852 | 1.00 | 46.29 |
| | 3630 | CB | GLU | 463 | 97.358 | 32.687 | 58.929 | 1.00 | 44.06 |
| | 3631 | CG | GLU | 463 | 96.076 | 33.063 | 59.677 | 1.00 | 51.03 |
| 40 | 3632 | CD | GLU | 463 | 96.101 | 32.673 | 61.150 | 1.00 | 55.15 |
| | 3633 | OE1 | GLU | 463 | 96.861 | 33.290 | 61.931 | 1.00 | 50.13 |
| | 3634 | OE2 | GLU | 463 | 95.348 | 31.752 | 61.529 | 1.00 | 55.86 |
| | 3635 | C | GLU | 463 | 96.530 | 30.483 | 58.041 | 1.00 | 44.39 |
| | 3636 | O | GLU | 463 | 95.690 | 29.774 | 58.600 | 1.00 | 47.37 |
| 45 | 3637 | N | CYS | 464 | 96.559 | 30.680 | 56.723 | 1.00 | 39.81 |
| | 3638 | CA | CYS | 464 | 95.589 | 30.068 | 55.816 | 1.00 | 37.44 |
| | 3639 | CB | CYS | 464 | 95.916 | 30.426 | 54.362 | 1.00 | 29.94 |
| | 3640 | SG | CYS | 464 | 95.879 | 32.186 | 53.990 | 1.00 | 33.66 |
| | 3641 | C | CYS | 464 | 95.630 | 28.556 | 55.973 | 1.00 | 39.78 |
| 50 | 3642 | O | CYS | 464 | 94.594 | 27.903 | 56.091 | 1.00 | 43.58 |
| | 3643 | N | CYS | 465 | 96.846 | 28.016 | 55.995 | 1.00 | 44.06 |

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|----|------|-----|-----|-----|--------|--------|--------|------|--------|
| | 3644 | CA | CYS | 465 | 97.072 | 26.583 | 56.133 | 1.00 | 43.89 |
| | 3645 | CB | CYS | 465 | 98.568 | 26.275 | 56.009 | 1.00 | 39.41 |
| | 3646 | SG | CYS | 465 | 98.961 | 24.513 | 55.936 | 1.00 | 40.79 |
| | 3647 | C | CYS | 465 | 96.532 | 26.052 | 57.454 | 1.00 | 44.77 |
| 5 | 3648 | O | CYS | 465 | 95.883 | 25.004 | 57.490 | 1.00 | 43.29 |
| | 3649 | N | MET | 466 | 96.788 | 26.794 | 58.530 | 1.00 | 50.46 |
| | 3650 | CA | MET | 466 | 96.342 | 26.418 | 59.870 | 1.00 | 59.83 |
| | 3651 | CB | MET | 466 | 96.838 | 27.429 | 60.916 | 1.00 | 58.39 |
| | 3652 | CG | MET | 466 | 98.343 | 27.424 | 61.149 | 1.00 | 55.57 |
| 10 | 3653 | SD | MET | 466 | 98.825 | 28.416 | 62.560 | 1.00 | 56.88 |
| | 3654 | CE | MET | 466 | 98.266 | 29.965 | 62.036 | 1.00 | 50.47 |
| | 3655 | C | MET | 466 | 94.825 | 26.271 | 59.979 | 1.00 | 64.16 |
| | 3656 | O | MET | 466 | 94.334 | 25.227 | 60.409 | 1.00 | 65.97 |
| | 3657 | N | ARG | 467 | 94.094 | 27.319 | 59.598 | 1.00 | 67.84 |
| 15 | 3658 | CA | ARG | 467 | 92.631 | 27.320 | 59.654 | 1.00 | 69.35 |
| | 3659 | CB | ARG | 467 | 92.083 | 28.744 | 59.512 | 1.00 | 75.34 |
| | 3660 | CG | ARG | 467 | 92.397 | 29.655 | 60.684 | 1.00 | 84.97 |
| | 3661 | CD | ARG | 467 | 91.640 | 30.965 | 60.560 | 1.00 | 96.41 |
| | 3662 | NE | ARG | 467 | 92.020 | 31.944 | 61.578 | 1.00 | 100.00 |
| 20 | 3663 | CZ | ARG | 467 | 91.475 | 33.152 | 61.696 | 1.00 | 100.00 |
| | 3664 | NH1 | ARG | 467 | 90.515 | 33.541 | 60.862 | 1.00 | 100.00 |
| | 3665 | NH2 | ARG | 467 | 91.901 | 33.982 | 62.639 | 1.00 | 100.00 |
| | 3666 | C | ARG | 467 | 91.965 | 26.415 | 58.620 | 1.00 | 64.55 |
| | 3667 | O | ARG | 467 | 90.863 | 25.907 | 58.853 | 1.00 | 66.78 |
| 25 | 3668 | N | ASP | 468 | 92.631 | 26.222 | 57.485 | 1.00 | 52.01 |
| | 3669 | CA | ASP | 468 | 92.108 | 25.383 | 56.412 | 1.00 | 45.50 |
| | 3670 | CB | ASP | 468 | 92.825 | 25.707 | 55.097 | 1.00 | 38.83 |
| | 3671 | CG | ASP | 468 | 92.140 | 25.103 | 53.886 | 1.00 | 38.56 |
| | 3672 | OD1 | ASP | 468 | 92.817 | 24.928 | 52.852 | 1.00 | 35.49 |
| 30 | 3673 | OD2 | ASP | 468 | 90.925 | 24.814 | 53.953 | 1.00 | 52.91 |
| | 3674 | C | ASP | 468 | 92.201 | 23.882 | 56.718 | 1.00 | 49.65 |
| | 3675 | O | ASP | 468 | 91.302 | 23.120 | 56.358 | 1.00 | 53.89 |
| | 3676 | N | TYR | 469 | 93.271 | 23.469 | 57.397 | 1.00 | 48.30 |
| | 3677 | CA | TYR | 469 | 93.475 | 22.059 | 57.740 | 1.00 | 47.34 |
| 35 | 3678 | CB | TYR | 469 | 94.887 | 21.611 | 57.345 | 1.00 | 49.69 |
| | 3679 | CG | TYR | 469 | 95.110 | 21.555 | 55.851 | 1.00 | 50.72 |
| | 3680 | CD1 | TYR | 469 | 95.085 | 20.339 | 55.169 | 1.00 | 53.63 |
| | 3681 | CE1 | TYR | 469 | 95.255 | 20.284 | 53.787 | 1.00 | 51.76 |
| | 3682 | CD2 | TYR | 469 | 95.318 | 22.719 | 55.113 | 1.00 | 50.18 |
| 40 | 3683 | CE2 | TYR | 469 | 95.489 | 22.675 | 53.732 | 1.00 | 50.61 |
| | 3684 | CZ | TYR | 469 | 95.455 | 21.456 | 53.075 | 1.00 | 54.80 |
| | 3685 | OH | TYR | 469 | 95.615 | 21.407 | 51.708 | 1.00 | 57.11 |
| | 3686 | C | TYR | 469 | 93.230 | 21.743 | 59.215 | 1.00 | 46.62 |
| | 3687 | O | TYR | 469 | 93.180 | 20.573 | 59.605 | 1.00 | 47.10 |
| 45 | 3688 | N | GLY | 470 | 93.069 | 22.788 | 60.026 | 1.00 | 43.51 |
| | 3689 | CA | GLY | 470 | 92.837 | 22.610 | 61.449 | 1.00 | 43.21 |
| | 3690 | C | GLY | 470 | 94.055 | 22.038 | 62.146 | 1.00 | 45.56 |
| | 3691 | O | GLY | 470 | 93.952 | 21.077 | 62.912 | 1.00 | 44.25 |
| | 3692 | N | ILE | 471 | 95.215 | 22.624 | 61.860 | 1.00 | 50.47 |
| 50 | 3693 | CA | ILE | 471 | 96.488 | 22.188 | 62.433 | 1.00 | 49.97 |

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|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 3694 | CB | ILE | 471 | 97.415 | 21.596 | 61.342 | 1.00 | 47.18 |
| | 3695 | CG2 | ILE | 471 | 96.844 | 20.285 | 60.811 | 1.00 | 47.32 |
| | 3696 | CG1 | ILE | 471 | 97.613 | 22.611 | 60.211 | 1.00 | 41.43 |
| | 3697 | CD1 | ILE | 471 | 98.427 | 22.094 | 59.049 | 1.00 | 46.18 |
| 5 | 3698 | C | ILE | 471 | 97.217 | 23.339 | 63.124 | 1.00 | 49.28 |
| | 3699 | O | ILE | 471 | 96.894 | 24.508 | 62.907 | 1.00 | 49.58 |
| | 3700 | N | SER | 472 | 98.204 | 23.000 | 63.949 | 1.00 | 49.04 |
| | 3701 | CA | SER | 472 | 98.986 | 23.998 | 64.674 | 1.00 | 52.64 |
| | 3702 | CB | SER | 472 | 99.748 | 23.340 | 65.829 | 1.00 | 54.48 |
| 10 | 3703 | OG | SER | 472 | 100.699 | 22.404 | 65.351 | 1.00 | 56.26 |
| | 3704 | C | SER | 472 | 99.969 | 24.716 | 63.753 | 1.00 | 53.26 |
| | 3705 | O | SER | 472 | 100.101 | 24.369 | 62.578 | 1.00 | 53.95 |
| | 3706 | N | THR | 473 | 100.650 | 25.725 | 64.292 | 1.00 | 53.55 |
| | 3707 | CA | THR | 473 | 101.634 | 26.491 | 63.531 | 1.00 | 54.18 |
| 15 | 3708 | CB | THR | 473 | 102.233 | 27.639 | 64.384 | 1.00 | 60.37 |
| | 3709 | OG1 | THR | 473 | 101.180 | 28.490 | 64.855 | 1.00 | 61.07 |
| | 3710 | CG2 | THR | 473 | 103.210 | 28.469 | 63.562 | 1.00 | 58.84 |
| | 3711 | C | THR | 473 | 102.760 | 25.550 | 63.105 | 1.00 | 51.25 |
| | 3712 | O | THR | 473 | 103.203 | 25.573 | 61.956 | 1.00 | 44.22 |
| 20 | 3713 | N | LYS | 474 | 103.173 | 24.697 | 64.038 | 1.00 | 49.57 |
| | 3714 | CA | LYS | 474 | 104.236 | 23.722 | 63.821 | 1.00 | 51.50 |
| | 3715 | CB | LYS | 474 | 104.440 | 22.903 | 65.098 | 1.00 | 55.84 |
| | 3716 | CG | LYS | 474 | 105.605 | 21.930 | 65.063 | 1.00 | 60.97 |
| | 3717 | CD | LYS | 474 | 105.778 | 21.266 | 66.421 | 1.00 | 66.81 |
| 25 | 3718 | CE | LYS | 474 | 107.011 | 20.382 | 66.462 | 1.00 | 71.89 |
| | 3719 | NZ | LYS | 474 | 107.261 | 19.853 | 67.832 | 1.00 | 72.76 |
| | 3720 | C | LYS | 474 | 103.924 | 22.797 | 62.646 | 1.00 | 53.47 |
| | 3721 | O | LYS | 474 | 104.759 | 22.603 | 61.759 | 1.00 | 56.55 |
| | 3722 | N | GLU | 475 | 102.712 | 22.249 | 62.637 | 1.00 | 54.30 |
| 30 | 3723 | CA | GLU | 475 | 102.271 | 21.342 | 61.578 | 1.00 | 54.12 |
| | 3724 | CB | GLU | 475 | 100.921 | 20.719 | 61.946 | 1.00 | 49.93 |
| | 3725 | CG | GLU | 475 | 100.940 | 19.925 | 63.244 | 1.00 | 54.09 |
| | 3726 | CD | GLU | 475 | 99.559 | 19.471 | 63.673 | 1.00 | 56.55 |
| | 3727 | OE1 | GLU | 475 | 99.055 | 18.476 | 63.111 | 1.00 | 59.40 |
| 35 | 3728 | OE2 | GLU | 475 | 98.977 | 20.109 | 64.577 | 1.00 | 54.88 |
| | 3729 | C | GLU | 475 | 102.170 | 22.043 | 60.224 | 1.00 | 48.29 |
| | 3730 | O | GLU | 475 | 102.514 | 21.465 | 59.192 | 1.00 | 43.53 |
| | 3731 | N | ALA | 476 | 101.706 | 23.291 | 60.240 | 1.00 | 47.85 |
| | 3732 | CA | ALA | 476 | 101.556 | 24.085 | 59.023 | 1.00 | 48.40 |
| 40 | 3733 | CB | ALA | 476 | 100.857 | 25.400 | 59.335 | 1.00 | 44.20 |
| | 3734 | C | ALA | 476 | 102.906 | 24.348 | 58.367 | 1.00 | 45.69 |
| | 3735 | O | ALA | 476 | 103.043 | 24.246 | 57.148 | 1.00 | 40.88 |
| | 3736 | N | MET | 477 | 103.897 | 24.690 | 59.185 | 1.00 | 46.31 |
| | 3737 | CA | MET | 477 | 105.241 | 24.956 | 58.687 | 1.00 | 47.60 |
| 45 | 3738 | CB | MET | 477 | 106.097 | 25.600 | 59.777 | 1.00 | 41.69 |
| | 3739 | CG | MET | 477 | 105.533 | 26.906 | 60.286 | 1.00 | 40.46 |
| | 3740 | SD | MET | 477 | 106.643 | 27.743 | 61.402 | 1.00 | 51.90 |
| | 3741 | CE | MET | 477 | 106.373 | 29.438 | 60.922 | 1.00 | 53.11 |
| | 3742 | C | MET | 477 | 105.882 | 23.659 | 58.213 | 1.00 | 47.15 |
| 50 | 3743 | O | MET | 477 | 106.580 | 23.637 | 57.196 | 1.00 | 43.34 |

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|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 3744 | N | ALA | 478 | 105.617 | 22.580 | 58.948 | 1.00 | 44.29 |
| | 3745 | CA | ALA | 478 | 106.146 | 21.262 | 58.617 | 1.00 | 43.92 |
| | 3746 | CB | ALA | 478 | 105.808 | 20.264 | 59.716 | 1.00 | 37.80 |
| | 3747 | C | ALA | 478 | 105.601 | 20.782 | 57.272 | 1.00 | 43.29 |
| 5 | 3748 | O | ALA | 478 | 106.312 | 20.127 | 56.509 | 1.00 | 44.64 |
| | 3749 | N | LYS | 479 | 104.346 | 21.116 | 56.981 | 1.00 | 45.34 |
| | 3750 | CA | LYS | 479 | 103.736 | 20.720 | 55.715 | 1.00 | 50.82 |
| | 3751 | CB | LYS | 479 | 102.214 | 20.847 | 55.762 | 1.00 | 57.75 |
| | 3752 | CG | LYS | 479 | 101.555 | 20.268 | 54.522 | 1.00 | 65.44 |
| 10 | 3753 | CD | LYS | 479 | 100.167 | 20.814 | 54.286 | 1.00 | 68.93 |
| | 3754 | CE | LYS | 479 | 99.651 | 20.332 | 52.943 | 1.00 | 68.91 |
| | 3755 | NZ | LYS | 479 | 98.384 | 20.999 | 52.566 | 1.00 | 74.62 |
| | 3756 | C | LYS | 479 | 104.283 | 21.581 | 54.581 | 1.00 | 47.22 |
| | 3757 | O | LYS | 479 | 104.451 | 21.109 | 53.455 | 1.00 | 50.00 |
| 15 | 3758 | N | PHE | 480 | 104.526 | 22.854 | 54.878 | 1.00 | 43.15 |
| | 3759 | CA | PHE | 480 | 105.076 | 23.776 | 53.894 | 1.00 | 41.41 |
| | 3760 | CB | PHE | 480 | 105.089 | 25.204 | 54.443 | 1.00 | 41.63 |
| | 3761 | CG | PHE | 480 | 103.894 | 26.021 | 54.033 | 1.00 | 44.23 |
| | 3762 | CD1 | PHE | 480 | 102.638 | 25.432 | 53.905 | 1.00 | 41.42 |
| 20 | 3763 | CD2 | PHE | 480 | 104.026 | 27.379 | 53.756 | 1.00 | 39.25 |
| | 3764 | CE1 | PHE | 480 | 101.535 | 26.182 | 53.503 | 1.00 | 36.23 |
| | 3765 | CE2 | PHE | 480 | 102.929 | 28.136 | 53.353 | 1.00 | 32.42 |
| | 3766 | CZ | PHE | 480 | 101.682 | 27.536 | 53.227 | 1.00 | 29.83 |
| | 3767 | C | PHE | 480 | 106.485 | 23.334 | 53.515 | 1.00 | 41.98 |
| 25 | 3768 | O | PHE | 480 | 106.881 | 23.434 | 52.353 | 1.00 | 37.95 |
| | 3769 | N | GLN | 481 | 107.229 | 22.824 | 54.495 | 1.00 | 41.79 |
| | 3770 | CA | GLN | 481 | 108.585 | 22.342 | 54.256 | 1.00 | 41.10 |
| | 3771 | CB | GLN | 481 | 109.236 | 21.868 | 55.559 | 1.00 | 39.98 |
| | 3772 | CG | GLN | 481 | 109.603 | 22.993 | 56.513 | 1.00 | 47.39 |
| 30 | 3773 | CD | GLN | 481 | 110.507 | 24.034 | 55.870 | 1.00 | 56.58 |
| | 3774 | OE1 | GLN | 481 | 111.605 | 23.720 | 55.406 | 1.00 | 55.49 |
| | 3775 | NE2 | GLN | 481 | 110.042 | 25.279 | 55.834 | 1.00 | 58.30 |
| | 3776 | C | GLN | 481 | 108.553 | 21.204 | 53.245 | 1.00 | 38.69 |
| | 3777 | O | GLN | 481 | 109.386 | 21.146 | 52.340 | 1.00 | 37.55 |
| 35 | 3778 | N | ASN | 482 | 107.564 | 20.324 | 53.391 | 1.00 | 35.14 |
| | 3779 | CA | ASN | 482 | 107.394 | 19.189 | 52.491 | 1.00 | 35.59 |
| | 3780 | CB | ASN | 482 | 106.302 | 18.250 | 53.009 | 1.00 | 41.18 |
| | 3781 | CG | ASN | 482 | 106.647 | 17.642 | 54.355 | 1.00 | 52.28 |
| | 3782 | OD1 | ASN | 482 | 107.756 | 17.148 | 54.560 | 1.00 | 53.57 |
| 40 | 3783 | ND2 | ASN | 482 | 105.697 | 17.678 | 55.282 | 1.00 | 61.08 |
| | 3784 | C | ASN | 482 | 107.057 | 19.657 | 51.081 | 1.00 | 32.00 |
| | 3785 | O | ASN | 482 | 107.358 | 18.971 | 50.105 | 1.00 | 35.80 |
| | 3786 | N | MET | 483 | 106.421 | 20.822 | 50.981 | 1.00 | 30.00 |
| | 3787 | CA | MET | 483 | 106.063 | 21.391 | 49.687 | 1.00 | 29.42 |
| 45 | 3788 | CB | MET | 483 | 105.092 | 22.562 | 49.855 | 1.00 | 33.61 |
| | 3789 | CG | MET | 483 | 103.693 | 22.173 | 50.303 | 1.00 | 33.22 |
| | 3790 | SD | MET | 483 | 102.589 | 23.605 | 50.374 | 1.00 | 34.18 |
| | 3791 | CE | MET | 483 | 102.294 | 23.881 | 48.638 | 1.00 | 31.57 |
| | 3792 | C | MET | 483 | 107.330 | 21.870 | 48.991 | 1.00 | 26.58 |
| 50 | 3793 | O | MET | 483 | 107.453 | 21.778 | 47.769 | 1.00 | 26.98 |

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|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 3794 | N | ALA | 484 | 108.267 | 22.386 | 49.782 | 1.00 | 24.14 |
| | 3795 | CA | ALA | 484 | 109.539 | 22.874 | 49.261 | 1.00 | 20.18 |
| | 3796 | CB | ALA | 484 | 110.260 | 23.687 | 50.323 | 1.00 | 15.48 |
| | 3797 | C | ALA | 484 | 110.399 | 21.694 | 48.812 | 1.00 | 18.99 |
| 5 | 3798 | O | ALA | 484 | 111.070 | 21.762 | 47.777 | 1.00 | 18.13 |
| | 3799 | N | GLU | 485 | 110.360 | 20.610 | 49.587 | 1.00 | 15.88 |
| | 3800 | CA | GLU | 485 | 111.115 | 19.398 | 49.274 | 1.00 | 22.72 |
| | 3801 | CB | GLU | 485 | 110.965 | 18.367 | 50.391 | 1.00 | 26.33 |
| | 3802 | CG | GLU | 485 | 111.571 | 18.811 | 51.719 | 1.00 | 57.96 |
| 10 | 3803 | CD | GLU | 485 | 111.355 | 17.814 | 52.853 | 1.00 | 66.33 |
| | 3804 | OE1 | GLU | 485 | 110.840 | 16.702 | 52.602 | 1.00 | 74.62 |
| | 3805 | OE2 | GLU | 485 | 111.704 | 18.149 | 54.006 | 1.00 | 72.14 |
| | 3806 | C | GLU | 485 | 110.625 | 18.806 | 47.962 | 1.00 | 19.07 |
| | 3807 | O | GLU | 485 | 111.422 | 18.403 | 47.114 | 1.00 | 23.09 |
| 15 | 3808 | N | THR | 486 | 109.306 | 18.768 | 47.802 | 1.00 | 18.34 |
| | 3809 | CA | THR | 486 | 108.680 | 18.247 | 46.594 | 1.00 | 13.68 |
| | 3810 | CB | THR | 486 | 107.132 | 18.239 | 46.724 | 1.00 | 19.42 |
| | 3811 | OG1 | THR | 486 | 106.740 | 17.320 | 47.753 | 1.00 | 18.34 |
| | 3812 | CG2 | THR | 486 | 106.474 | 17.832 | 45.409 | 1.00 | 7.13 |
| 20 | 3813 | C | THR | 486 | 109.084 | 19.126 | 45.418 | 1.00 | 12.40 |
| | 3814 | O | THR | 486 | 109.432 | 18.628 | 44.347 | 1.00 | 12.64 |
| | 3815 | N | ALA | 487 | 109.054 | 20.437 | 45.641 | 1.00 | 18.37 |
| | 3816 | CA | ALA | 487 | 109.420 | 21.406 | 44.618 | 1.00 | 14.12 |
| | 3817 | CB | ALA | 487 | 109.224 | 22.812 | 45.137 | 1.00 | 12.83 |
| 25 | 3818 | C | ALA | 487 | 110.863 | 21.195 | 44.178 | 1.00 | 11.72 |
| | 3819 | O | ALA | 487 | 111.182 | 21.312 | 42.993 | 1.00 | 14.71 |
| | 3820 | N | TRP | 488 | 111.731 | 20.860 | 45.128 | 1.00 | 11.21 |
| | 3821 | CA | TRP | 488 | 113.129 | 20.616 | 44.801 | 1.00 | 9.46 |
| | 3822 | CB | TRP | 488 | 113.985 | 20.541 | 46.061 | 1.00 | 2.00 |
| 30 | 3823 | CG | TRP | 488 | 114.586 | 21.864 | 46.394 | 1.00 | 10.22 |
| | 3824 | CD2 | TRP | 488 | 115.535 | 22.596 | 45.602 | 1.00 | 8.75 |
| | 3825 | CE2 | TRP | 488 | 115.798 | 23.807 | 46.279 | 1.00 | 8.09 |
| | 3826 | CE3 | TRP | 488 | 116.186 | 22.345 | 44.384 | 1.00 | 8.76 |
| | 3827 | CD1 | TRP | 488 | 114.322 | 22.636 | 47.488 | 1.00 | 2.81 |
| 35 | 3828 | NE1 | TRP | 488 | 115.045 | 23.807 | 47.425 | 1.00 | 14.28 |
| | 3829 | CZ2 | TRP | 488 | 116.686 | 24.768 | 45.780 | 1.00 | 4.43 |
| | 3830 | CZ3 | TRP | 488 | 117.072 | 23.301 | 43.885 | 1.00 | 8.98 |
| | 3831 | CH2 | TRP | 488 | 117.312 | 24.497 | 44.585 | 1.00 | 9.72 |
| | 3832 | C | TRP | 488 | 113.306 | 19.378 | 43.936 | 1.00 | 9.87 |
| 40 | 3833 | O | TRP | 488 | 114.112 | 19.380 | 43.005 | 1.00 | 11.24 |
| | 3834 | N | LYS | 489 | 112.526 | 18.335 | 44.214 | 1.00 | 7.93 |
| | 3835 | CA | LYS | 489 | 112.601 | 17.110 | 43.427 | 1.00 | 2.00 |
| | 3836 | CB | LYS | 489 | 111.815 | 15.987 | 44.096 | 1.00 | 7.82 |
| | 3837 | CG | LYS | 489 | 112.350 | 15.603 | 45.470 | 1.00 | 9.24 |
| 45 | 3838 | CD | LYS | 489 | 111.550 | 14.471 | 46.069 | 1.00 | 2.14 |
| | 3839 | CE | LYS | 489 | 111.921 | 14.248 | 47.517 | 1.00 | 16.24 |
| | 3840 | NZ | LYS | 489 | 111.056 | 13.208 | 48.146 | 1.00 | 26.26 |
| | 3841 | C | LYS | 489 | 112.051 | 17.390 | 42.037 | 1.00 | 7.99 |
| | 3842 | O | LYS | 489 | 112.480 | 16.784 | 41.055 | 1.00 | 11.24 |
| 50 | 3843 | N | ASP | 490 | 111.115 | 18.333 | 41.960 | 1.00 | 9.24 |

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|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 3844 | CA | ASP | 490 | 110.518 | 18.716 | 40.687 | 1.00 | 12.50 |
| | 3845 | CB | ASP | 490 | 109.234 | 19.514 | 40.901 | 1.00 | 15.83 |
| | 3846 | CG | ASP | 490 | 108.083 | 18.648 | 41.360 | 1.00 | 23.66 |
| | 3847 | OD1 | ASP | 490 | 107.949 | 17.509 | 40.856 | 1.00 | 20.17 |
| 5 | 3848 | OD2 | ASP | 490 | 107.308 | 19.111 | 42.221 | 1.00 | 28.73 |
| | 3849 | C | ASP | 490 | 111.501 | 19.522 | 39.856 | 1.00 | 11.20 |
| | 3850 | O | ASP | 490 | 111.519 | 19.409 | 38.629 | 1.00 | 17.78 |
| | 3851 | N | ILE | 491 | 112.308 | 20.345 | 40.523 | 1.00 | 16.49 |
| | 3852 | CA | ILE | 491 | 113.311 | 21.149 | 39.831 | 1.00 | 15.96 |
| 10 | 3853 | CB | ILE | 491 | 113.973 | 22.183 | 40.766 | 1.00 | 14.10 |
| | 3854 | CG2 | ILE | 491 | 115.138 | 22.870 | 40.058 | 1.00 | 17.39 |
| | 3855 | CG1 | ILE | 491 | 112.938 | 23.221 | 41.209 | 1.00 | 20.61 |
| | 3856 | CD1 | ILE | 491 | 113.493 | 24.319 | 42.097 | 1.00 | 6.59 |
| | 3857 | C | ILE | 491 | 114.372 | 20.207 | 39.279 | 1.00 | 11.72 |
| 15 | 3858 | O | ILE | 491 | 114.802 | 20.342 | 38.132 | 1.00 | 18.27 |
| | 3859 | N | ASN | 492 | 114.744 | 19.217 | 40.084 | 1.00 | 9.30 |
| | 3860 | CA | ASN | 492 | 115.739 | 18.232 | 39.684 | 1.00 | 8.49 |
| | 3861 | CB | ASN | 492 | 116.078 | 17.320 | 40.866 | 1.00 | 8.53 |
| | 3862 | CG | ASN | 492 | 116.793 | 18.062 | 41.986 | 1.00 | 2.00 |
| 20 | 3863 | OD1 | ASN | 492 | 117.444 | 19.081 | 41.756 | 1.00 | 2.00 |
| | 3864 | ND2 | ASN | 492 | 116.674 | 17.554 | 43.204 | 1.00 | 9.30 |
| | 3865 | C | ASN | 492 | 115.296 | 17.421 | 38.458 | 1.00 | 6.69 |
| | 3866 | O | ASN | 492 | 116.120 | 17.067 | 37.618 | 1.00 | 15.10 |
| | 3867 | N | GLU | 493 | 113.994 | 17.157 | 38.345 | 1.00 | 11.11 |
| 25 | 3868 | CA | GLU | 493 | 113.452 | 16.420 | 37.203 | 1.00 | 6.79 |
| | 3869 | CB | GLU | 493 | 112.036 | 15.929 | 37.490 | 1.00 | 14.43 |
| | 3870 | CG | GLU | 493 | 111.966 | 14.681 | 38.344 | 1.00 | 35.11 |
| | 3871 | CD | GLU | 493 | 110.554 | 14.143 | 38.504 | 1.00 | 39.54 |
| | 3872 | OE1 | GLU | 493 | 109.669 | 14.505 | 37.695 | 1.00 | 36.96 |
| 30 | 3873 | OE2 | GLU | 493 | 110.335 | 13.345 | 39.441 | 1.00 | 44.74 |
| | 3874 | C | GLU | 493 | 113.420 | 17.284 | 35.947 | 1.00 | 15.20 |
| | 3875 | O | GLU | 493 | 113.539 | 16.777 | 34.828 | 1.00 | 19.79 |
| | 3876 | N | GLY | 494 | 113.234 | 18.588 | 36.140 | 1.00 | 15.92 |
| 35 | 3877 | CA | GLY | 494 | 113.176 | 19.512 | 35.021 | 1.00 | 13.61 |
| | 3878 | C | GLY | 494 | 114.488 | 19.613 | 34.276 | 1.00 | 18.91 |
| | 3879 | O | GLY | 494 | 114.507 | 19.822 | 33.061 | 1.00 | 23.19 |
| | 3880 | N | LEU | 495 | 115.583 | 19.437 | 35.008 | 1.00 | 18.93 |
| | 3881 | CA | LEU | 495 | 116.927 | 19.508 | 34.445 | 1.00 | 18.10 |
| | 3882 | CB | LEU | 495 | 117.955 | 19.662 | 35.571 | 1.00 | 12.15 |
| 40 | 3883 | CG | LEU | 495 | 117.764 | 20.846 | 36.527 | 1.00 | 11.37 |
| | 3884 | CD1 | LEU | 495 | 118.788 | 20.781 | 37.650 | 1.00 | 2.00 |
| | 3885 | CD2 | LEU | 495 | 117.866 | 22.164 | 35.771 | 1.00 | 6.14 |
| | 3886 | C | LEU | 495 | 117.279 | 18.289 | 33.593 | 1.00 | 21.97 |
| | 3887 | O | LEU | 495 | 118.146 | 18.366 | 32.717 | 1.00 | 20.13 |
| 45 | 3888 | N | LEU | 496 | 116.602 | 17.171 | 33.849 | 1.00 | 21.91 |
| | 3889 | CA | LEU | 496 | 116.851 | 15.931 | 33.118 | 1.00 | 15.41 |
| | 3890 | CB | LEU | 496 | 116.126 | 14.760 | 33.784 | 1.00 | 8.37 |
| | 3891 | CG | LEU | 496 | 116.604 | 14.435 | 35.204 | 1.00 | 10.05 |
| | 3892 | CD1 | LEU | 496 | 115.819 | 13.269 | 35.769 | 1.00 | 2.00 |
| 50 | 3893 | CD2 | LEU | 496 | 118.094 | 14.121 | 35.206 | 1.00 | 5.54 |

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|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 3894 | C | LEU | 496 | 116.492 | 16.017 | 31.641 | 1.00 | 14.28 |
| | 3895 | O | LEU | 496 | 115.471 | 16.593 | 31.269 | 1.00 | 19.94 |
| | 3896 | N | ARG | 497 | 117.360 | 15.454 | 30.808 | 1.00 | 16.05 |
| | 3897 | CA | ARG | 497 | 117.184 | 15.456 | 29.359 | 1.00 | 18.50 |
| 5 | 3898 | CB | ARG | 497 | 118.516 | 15.107 | 28.682 | 1.00 | 19.50 |
| | 3899 | CG | ARG | 497 | 119.665 | 16.035 | 29.066 | 1.00 | 28.42 |
| | 3900 | CD | ARG | 497 | 121.024 | 15.363 | 28.908 | 1.00 | 24.39 |
| | 3901 | NE | ARG | 497 | 121.803 | 15.905 | 27.797 | 1.00 | 27.16 |
| | 3902 | CZ | ARG | 497 | 122.978 | 16.517 | 27.927 | 1.00 | 26.59 |
| 10 | 3903 | NH1 | ARG | 497 | 123.525 | 16.677 | 29.125 | 1.00 | 14.53 |
| | 3904 | NH2 | ARG | 497 | 123.618 | 16.955 | 26.850 | 1.00 | 32.59 |
| | 3905 | C | ARG | 497 | 116.099 | 14.471 | 28.922 | 1.00 | 23.25 |
| | 3906 | O | ARG | 497 | 115.890 | 13.441 | 29.566 | 1.00 | 25.86 |
| | 3907 | N | PRO | 498 | 115.369 | 14.793 | 27.838 | 1.00 | 22.25 |
| 15 | 3908 | CD | PRO | 498 | 114.524 | 13.808 | 27.150 | 1.00 | 25.52 |
| | 3909 | CA | PRO | 498 | 115.491 | 16.003 | 27.017 | 1.00 | 25.55 |
| | 3910 | CB | PRO | 498 | 114.781 | 15.612 | 25.715 | 1.00 | 17.40 |
| | 3911 | CG | PRO | 498 | 114.819 | 14.122 | 25.715 | 1.00 | 25.69 |
| | 3912 | C | PRO | 498 | 114.785 | 17.192 | 27.662 | 1.00 | 28.98 |
| 20 | 3913 | O | PRO | 498 | 113.609 | 17.104 | 28.021 | 1.00 | 33.06 |
| | 3914 | N | THR | 499 | 115.506 | 18.299 | 27.804 | 1.00 | 24.14 |
| | 3915 | CA | THR | 499 | 114.949 | 19.511 | 28.391 | 1.00 | 15.92 |
| | 3916 | CB | THR | 499 | 116.070 | 20.473 | 28.835 | 1.00 | 16.49 |
| | 3917 | OG1 | THR | 499 | 116.946 | 20.735 | 27.730 | 1.00 | 6.47 |
| 25 | 3918 | CG2 | THR | 499 | 116.870 | 19.862 | 29.983 | 1.00 | 10.26 |
| | 3919 | C | THR | 499 | 114.043 | 20.205 | 27.374 | 1.00 | 19.26 |
| | 3920 | O | THR | 499 | 114.329 | 20.205 | 26.174 | 1.00 | 30.87 |
| | 3921 | N | PRO | 500 | 112.919 | 20.776 | 27.836 | 1.00 | 16.60 |
| | 3922 | CD | PRO | 500 | 112.472 | 20.794 | 29.239 | 1.00 | 9.65 |
| 30 | 3923 | CA | PRO | 500 | 111.959 | 21.473 | 26.971 | 1.00 | 19.15 |
| | 3924 | CB | PRO | 500 | 110.870 | 21.907 | 27.954 | 1.00 | 16.41 |
| | 3925 | CG | PRO | 500 | 111.599 | 22.004 | 29.267 | 1.00 | 14.64 |
| | 3926 | C | PRO | 500 | 112.569 | 22.656 | 26.213 | 1.00 | 26.43 |
| | 3927 | O | PRO | 500 | 112.131 | 23.001 | 25.111 | 1.00 | 28.97 |
| 35 | 3928 | N | VAL | 501 | 113.580 | 23.266 | 26.824 | 1.00 | 27.74 |
| | 3929 | CA | VAL | 501 | 114.317 | 24.393 | 26.253 | 1.00 | 27.33 |
| | 3930 | CB | VAL | 501 | 113.874 | 25.749 | 26.867 | 1.00 | 25.49 |
| | 3931 | CG1 | VAL | 501 | 112.495 | 26.136 | 26.367 | 1.00 | 27.78 |
| | 3932 | CG2 | VAL | 501 | 113.880 | 25.675 | 28.386 | 1.00 | 25.11 |
| 40 | 3933 | C | VAL | 501 | 115.792 | 24.149 | 26.572 | 1.00 | 27.50 |
| | 3934 | O | VAL | 501 | 116.118 | 23.190 | 27.268 | 1.00 | 34.26 |
| | 3935 | N | SER | 502 | 116.685 | 24.991 | 26.059 | 1.00 | 27.56 |
| | 3936 | CA | SER | 502 | 118.111 | 24.821 | 26.336 | 1.00 | 26.62 |
| | 3937 | CB | SER | 502 | 118.942 | 25.802 | 25.513 | 1.00 | 31.78 |
| 45 | 3938 | OG | SER | 502 | 118.853 | 25.497 | 24.133 | 1.00 | 55.84 |
| | 3939 | C | SER | 502 | 118.407 | 25.000 | 27.823 | 1.00 | 30.86 |
| | 3940 | O | SER | 502 | 117.759 | 25.801 | 28.505 | 1.00 | 31.25 |
| | 3941 | N | THR | 503 | 119.387 | 24.247 | 28.318 | 1.00 | 31.45 |
| | 3942 | CA | THR | 503 | 119.785 | 24.296 | 29.726 | 1.00 | 32.20 |
| 50 | 3943 | CB | THR | 503 | 121.008 | 23.389 | 29.989 | 1.00 | 33.25 |

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|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 3944 | OG1 | THR | 503 | 120.732 | 22.067 | 29.511 | 1.00 | 46.44 |
| | 3945 | CG2 | THR | 503 | 121.316 | 23.320 | 31.478 | 1.00 | 33.35 |
| | 3946 | C | THR | 503 | 120.119 | 25.722 | 30.162 | 1.00 | 25.43 |
| 5 | 3947 | O | THR | 503 | 119.955 | 26.087 | 31.331 | 1.00 | 17.17 |
| | 3948 | N | GLU | 504 | 120.569 | 26.522 | 29.200 | 1.00 | 21.60 |
| | 3949 | CA | GLU | 504 | 120.931 | 27.914 | 29.433 | 1.00 | 21.35 |
| | 3950 | CB | GLU | 504 | 121.355 | 28.549 | 28.104 | 1.00 | 16.54 |
| | 3951 | CG | GLU | 504 | 121.779 | 30.009 | 28.189 | 1.00 | 26.78 |
| 10 | 3952 | CD | GLU | 504 | 122.043 | 30.642 | 26.825 | 1.00 | 35.29 |
| | 3953 | OE1 | GLU | 504 | 121.832 | 29.971 | 25.789 | 1.00 | 38.25 |
| | 3954 | OE2 | GLU | 504 | 122.460 | 31.821 | 26.793 | 1.00 | 34.16 |
| | 3955 | C | GLU | 504 | 119.747 | 28.680 | 30.028 | 1.00 | 20.56 |
| | 3956 | O | GLU | 504 | 119.924 | 29.595 | 30.837 | 1.00 | 14.15 |
| 15 | 3957 | N | PHE | 505 | 118.541 | 28.251 | 29.665 | 1.00 | 18.81 |
| | 3958 | CA | PHE | 505 | 117.320 | 28.896 | 30.126 | 1.00 | 15.87 |
| | 3959 | CB | PHE | 505 | 116.330 | 28.995 | 28.966 | 1.00 | 13.36 |
| | 3960 | CG | PHE | 505 | 116.892 | 29.710 | 27.769 | 1.00 | 20.57 |
| | 3961 | CD1 | PHE | 505 | 117.193 | 29.013 | 26.602 | 1.00 | 24.10 |
| | 3962 | CD2 | PHE | 505 | 117.183 | 31.070 | 27.831 | 1.00 | 20.76 |
| 20 | 3963 | CE1 | PHE | 505 | 117.782 | 29.658 | 25.517 | 1.00 | 19.64 |
| | 3964 | CE2 | PHE | 505 | 117.772 | 31.724 | 26.754 | 1.00 | 25.52 |
| | 3965 | CZ | PHE | 505 | 118.072 | 31.015 | 25.595 | 1.00 | 26.72 |
| | 3966 | C | PHE | 505 | 116.675 | 28.274 | 31.358 | 1.00 | 15.98 |
| | 3967 | O | PHE | 505 | 115.703 | 28.808 | 31.886 | 1.00 | 16.03 |
| 25 | 3968 | N | LEU | 506 | 117.232 | 27.162 | 31.829 | 1.00 | 16.47 |
| | 3969 | CA | LEU | 506 | 116.712 | 26.492 | 33.018 | 1.00 | 10.03 |
| | 3970 | CB | LEU | 506 | 116.774 | 24.972 | 32.856 | 1.00 | 19.45 |
| | 3971 | CG | LEU | 506 | 115.962 | 24.330 | 31.729 | 1.00 | 25.84 |
| | 3972 | CD1 | LEU | 506 | 116.268 | 22.852 | 31.690 | 1.00 | 29.46 |
| 30 | 3973 | CD2 | LEU | 506 | 114.473 | 24.557 | 31.928 | 1.00 | 24.50 |
| | 3974 | C | LEU | 506 | 117.503 | 26.895 | 34.254 | 1.00 | 11.68 |
| | 3975 | O | LEU | 506 | 116.967 | 26.926 | 35.365 | 1.00 | 15.18 |
| | 3976 | N | THR | 507 | 118.781 | 27.210 | 34.054 | 1.00 | 10.27 |
| | 3977 | CA | THR | 507 | 119.662 | 27.601 | 35.151 | 1.00 | 7.47 |
| 35 | 3978 | CB | THR | 507 | 121.108 | 27.838 | 34.671 | 1.00 | 10.86 |
| | 3979 | OG1 | THR | 507 | 121.492 | 26.798 | 33.762 | 1.00 | 20.06 |
| | 3980 | CG2 | THR | 507 | 122.058 | 27.824 | 35.852 | 1.00 | 2.66 |
| | 3981 | C | THR | 507 | 119.181 | 28.824 | 35.936 | 1.00 | 10.65 |
| | 3982 | O | THR | 507 | 119.229 | 28.821 | 37.167 | 1.00 | 14.58 |
| 40 | 3983 | N | PRO | 508 | 118.718 | 29.887 | 35.242 | 1.00 | 8.73 |
| | 3984 | CD | PRO | 508 | 118.680 | 30.110 | 33.784 | 1.00 | 7.34 |
| | 3985 | CA | PRO | 508 | 118.244 | 31.080 | 35.956 | 1.00 | 5.70 |
| | 3986 | CB | PRO | 508 | 117.717 | 31.959 | 34.826 | 1.00 | 8.88 |
| | 3987 | CG | PRO | 508 | 118.630 | 31.616 | 33.688 | 1.00 | 2.00 |
| 45 | 3988 | C | PRO | 508 | 117.141 | 30.742 | 36.955 | 1.00 | 16.13 |
| | 3989 | O | PRO | 508 | 117.109 | 31.282 | 38.064 | 1.00 | 19.06 |
| | 3990 | N | ILE | 509 | 116.254 | 29.831 | 36.555 | 1.00 | 12.82 |
| | 3991 | CA | ILE | 509 | 115.149 | 29.390 | 37.401 | 1.00 | 7.60 |
| | 3992 | CB | ILE | 509 | 114.201 | 28.444 | 36.635 | 1.00 | 13.85 |
| 50 | 3993 | CG2 | ILE | 509 | 113.160 | 27.865 | 37.577 | 1.00 | 3.89 |

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|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 3994 | CG1 | ILE | 509 | 113.533 | 29.189 | 35.477 | 1.00 | 8.63 |
| | 3995 | CD1 | ILE | 509 | 112.681 | 28.301 | 34.597 | 1.00 | 16.09 |
| | 3996 | C | ILE | 509 | 115.723 | 28.657 | 38.604 | 1.00 | 10.09 |
| | 3997 | O | ILE | 509 | 115.320 | 28.906 | 39.744 | 1.00 | 13.81 |
| 5 | 3998 | N | LEU | 510 | 116.670 | 27.759 | 38.335 | 1.00 | 10.69 |
| | 3999 | CA | LEU | 510 | 117.347 | 26.983 | 39.376 | 1.00 | 8.28 |
| | 4000 | CB | LEU | 510 | 118.381 | 26.047 | 38.738 | 1.00 | 13.30 |
| | 4001 | CG | LEU | 510 | 119.429 | 25.349 | 39.612 | 1.00 | 10.83 |
| | 4002 | CD1 | LEU | 510 | 118.781 | 24.553 | 40.736 | 1.00 | 9.01 |
| 10 | 4003 | CD2 | LEU | 510 | 120.267 | 24.444 | 38.728 | 1.00 | 2.40 |
| | 4004 | C | LEU | 510 | 118.033 | 27.927 | 40.358 | 1.00 | 4.13 |
| | 4005 | O | LEU | 510 | 117.860 | 27.806 | 41.570 | 1.00 | 2.43 |
| | 4006 | N | ASN | 511 | 118.778 | 28.890 | 39.819 | 1.00 | 12.14 |
| | 4007 | CA | ASN | 511 | 119.487 | 29.875 | 40.627 | 1.00 | 11.57 |
| 15 | 4008 | CB | ASN | 511 | 120.347 | 30.773 | 39.743 | 1.00 | 12.88 |
| | 4009 | CG | ASN | 511 | 121.567 | 30.054 | 39.208 | 1.00 | 18.35 |
| | 4010 | OD1 | ASN | 511 | 122.137 | 29.196 | 39.881 | 1.00 | 15.86 |
| | 4011 | ND2 | ASN | 511 | 121.972 | 30.396 | 37.991 | 1.00 | 27.20 |
| | 4012 | C | ASN | 511 | 118.553 | 30.710 | 41.487 | 1.00 | 11.23 |
| 20 | 4013 | O | ASN | 511 | 118.883 | 31.018 | 42.634 | 1.00 | 9.07 |
| | 4014 | N | LEU | 512 | 117.387 | 31.058 | 40.941 | 1.00 | 13.33 |
| | 4015 | CA | LEU | 512 | 116.393 | 31.837 | 41.683 | 1.00 | 8.79 |
| | 4016 | CB | LEU | 512 | 115.168 | 32.131 | 40.814 | 1.00 | 13.75 |
| | 4017 | CG | LEU | 512 | 115.255 | 33.332 | 39.865 | 1.00 | 12.09 |
| 25 | 4018 | CD1 | LEU | 512 | 114.100 | 33.306 | 38.884 | 1.00 | 2.00 |
| | 4019 | CD2 | LEU | 512 | 115.256 | 34.623 | 40.667 | 1.00 | 2.00 |
| | 4020 | C | LEU | 512 | 115.975 | 31.083 | 42.940 | 1.00 | 10.14 |
| | 4021 | O | LEU | 512 | 115.810 | 31.682 | 44.002 | 1.00 | 13.04 |
| | 4022 | N | ALA | 513 | 115.836 | 29.764 | 42.819 | 1.00 | 10.74 |
| 30 | 4023 | CA | ALA | 513 | 115.464 | 28.916 | 43.951 | 1.00 | 12.16 |
| | 4024 | CB | ALA | 513 | 115.097 | 27.523 | 43.464 | 1.00 | 14.93 |
| | 4025 | C | ALA | 513 | 116.621 | 28.842 | 44.947 | 1.00 | 13.31 |
| | 4026 | O | ALA | 513 | 116.408 | 28.757 | 46.157 | 1.00 | 9.13 |
| | 4027 | N | ARG | 514 | 117.846 | 28.879 | 44.424 | 1.00 | 19.25 |
| 35 | 4028 | CA | ARG | 514 | 119.048 | 28.834 | 45.253 | 1.00 | 17.40 |
| | 4029 | CB | ARG | 514 | 120.294 | 28.644 | 44.382 | 1.00 | 14.56 |
| | 4030 | CG | ARG | 514 | 120.493 | 27.229 | 43.863 | 1.00 | 4.10 |
| | 4031 | CD | ARG | 514 | 121.602 | 27.170 | 42.823 | 1.00 | 9.06 |
| | 4032 | NE | ARG | 514 | 121.943 | 25.793 | 42.471 | 1.00 | 17.13 |
| 40 | 4033 | CZ | ARG | 514 | 122.653 | 25.434 | 41.403 | 1.00 | 16.59 |
| | 4034 | NH1 | ARG | 514 | 123.107 | 26.346 | 40.554 | 1.00 | 8.47 |
| | 4035 | NH2 | ARG | 514 | 122.929 | 24.154 | 41.197 | 1.00 | 15.58 |
| | 4036 | C | ARG | 514 | 119.190 | 30.106 | 46.084 | 1.00 | 13.80 |
| | 4037 | O | ARG | 514 | 119.522 | 30.051 | 47.270 | 1.00 | 10.51 |
| 45 | 4038 | N | ILE | 515 | 118.901 | 31.247 | 45.466 | 1.00 | 15.59 |
| | 4039 | CA | ILE | 515 | 119.011 | 32.535 | 46.147 | 1.00 | 20.36 |
| | 4040 | CB | ILE | 515 | 118.764 | 33.718 | 45.194 | 1.00 | 12.70 |
| | 4041 | CG2 | ILE | 515 | 119.221 | 35.007 | 45.851 | 1.00 | 25.50 |
| | 4042 | CG1 | ILE | 515 | 119.567 | 33.534 | 43.910 | 1.00 | 19.52 |
| 50 | 4043 | CD1 | ILE | 515 | 119.220 | 34.523 | 42.828 | 1.00 | 29.86 |

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|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 4044 | C | ILE | 515 | 118.085 | 32.672 | 47.353 | 1.00 | 17.44 |
| | 4045 | O | ILE | 515 | 118.477 | 33.257 | 48.359 | 1.00 | 19.69 |
| | 4046 | N | VAL | 516 | 116.868 | 32.136 | 47.258 | 1.00 | 21.26 |
| | 4047 | CA | VAL | 516 | 115.915 | 32.218 | 48.369 | 1.00 | 23.09 |
| 5 | 4048 | CB | VAL | 516 | 114.504 | 31.679 | 48.008 | 1.00 | 32.21 |
| | 4049 | CG1 | VAL | 516 | 113.444 | 32.441 | 48.787 | 1.00 | 27.43 |
| | 4050 | CG2 | VAL | 516 | 114.244 | 31.755 | 46.526 | 1.00 | 29.34 |
| | 4051 | C | VAL | 516 | 116.424 | 31.382 | 49.535 | 1.00 | 20.14 |
| | 4052 | O | VAL | 516 | 116.429 | 31.835 | 50.681 | 1.00 | 22.46 |
| 10 | 4053 | N | GLU | 517 | 116.833 | 30.154 | 49.229 | 1.00 | 21.26 |
| | 4054 | CA | GLU | 517 | 117.352 | 29.230 | 50.231 | 1.00 | 23.87 |
| | 4055 | CB | GLU | 517 | 117.859 | 27.949 | 49.555 | 1.00 | 24.13 |
| | 4056 | CG | GLU | 517 | 116.765 | 27.008 | 49.049 | 1.00 | 27.64 |
| | 4057 | CD | GLU | 517 | 116.153 | 26.132 | 50.143 | 1.00 | 36.07 |
| 15 | 4058 | OE1 | GLU | 517 | 116.480 | 26.314 | 51.336 | 1.00 | 40.38 |
| | 4059 | OE2 | GLU | 517 | 115.338 | 25.248 | 49.804 | 1.00 | 38.38 |
| | 4060 | C | GLU | 517 | 118.484 | 29.872 | 51.024 | 1.00 | 25.33 |
| | 4061 | O | GLU | 517 | 118.488 | 29.840 | 52.255 | 1.00 | 28.96 |
| | 4062 | N | VAL | 518 | 119.411 | 30.492 | 50.297 | 1.00 | 22.43 |
| 20 | 4063 | CA | VAL | 518 | 120.577 | 31.156 | 50.874 | 1.00 | 22.95 |
| | 4064 | CB | VAL | 518 | 121.605 | 31.482 | 49.762 | 1.00 | 24.42 |
| | 4065 | CG1 | VAL | 518 | 122.767 | 32.289 | 50.313 | 1.00 | 23.12 |
| | 4066 | CG2 | VAL | 518 | 122.105 | 30.194 | 49.125 | 1.00 | 20.43 |
| | 4067 | C | VAL | 518 | 120.239 | 32.436 | 51.649 | 1.00 | 24.42 |
| 25 | 4068 | O | VAL | 518 | 120.850 | 32.725 | 52.683 | 1.00 | 23.34 |
| | 4069 | N | THR | 519 | 119.267 | 33.192 | 51.145 | 1.00 | 22.60 |
| | 4070 | CA | THR | 519 | 118.846 | 34.443 | 51.769 | 1.00 | 20.24 |
| | 4071 | CB | THR | 519 | 118.044 | 35.305 | 50.773 | 1.00 | 23.46 |
| | 4072 | OG1 | THR | 519 | 118.872 | 35.615 | 49.646 | 1.00 | 23.28 |
| 30 | 4073 | CG2 | THR | 519 | 117.597 | 36.601 | 51.410 | 1.00 | 22.46 |
| | 4074 | C | THR | 519 | 118.051 | 34.232 | 53.058 | 1.00 | 25.34 |
| | 4075 | O | THR | 519 | 118.164 | 35.020 | 54.000 | 1.00 | 24.48 |
| | 4076 | N | TYR | 520 | 117.261 | 33.162 | 53.105 | 1.00 | 30.17 |
| | 4077 | CA | TYR | 520 | 116.461 | 32.848 | 54.290 | 1.00 | 34.43 |
| 35 | 4078 | CB | TYR | 520 | 115.017 | 32.528 | 53.892 | 1.00 | 35.49 |
| | 4079 | CG | TYR | 520 | 114.238 | 33.696 | 53.330 | 1.00 | 32.60 |
| | 4080 | CD1 | TYR | 520 | 114.481 | 34.171 | 52.041 | 1.00 | 27.24 |
| | 4081 | CE1 | TYR | 520 | 113.758 | 35.242 | 51.520 | 1.00 | 34.38 |
| | 4082 | CD2 | TYR | 520 | 113.247 | 34.321 | 54.087 | 1.00 | 30.57 |
| 40 | 4083 | CE2 | TYR | 520 | 112.516 | 35.392 | 53.577 | 1.00 | 22.83 |
| | 4084 | CZ | TYR | 520 | 112.777 | 35.848 | 52.294 | 1.00 | 34.91 |
| | 4085 | OH | TYR | 520 | 112.070 | 36.916 | 51.787 | 1.00 | 38.85 |
| | 4086 | C | TYR | 520 | 117.047 | 31.663 | 55.058 | 1.00 | 37.02 |
| | 4087 | O | TYR | 520 | 116.321 | 30.937 | 55.740 | 1.00 | 41.01 |
| 45 | 4088 | N | ILE | 521 | 118.361 | 31.483 | 54.956 | 1.00 | 39.45 |
| | 4089 | CA | ILE | 521 | 119.048 | 30.380 | 55.621 | 1.00 | 41.53 |
| | 4090 | CB | ILE | 521 | 120.561 | 30.363 | 55.251 | 1.00 | 34.97 |
| | 4091 | CG2 | ILE | 521 | 121.263 | 31.607 | 55.775 | 1.00 | 33.59 |
| | 4092 | CG1 | ILE | 521 | 121.228 | 29.087 | 55.770 | 1.00 | 32.90 |
| 50 | 4093 | CD1 | ILE | 521 | 122.620 | 28.865 | 55.224 | 1.00 | 16.56 |

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|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 4094 | C | ILE | 521 | 118.841 | 30.384 | 57.140 | 1.00 | 51.61 |
| | 4095 | O | ILE | 521 | 118.649 | 29.329 | 57.750 | 1.00 | 55.56 |
| | 4096 | N | HIS | 522 | 118.840 | 31.573 | 57.737 | 1.00 | 57.98 |
| | 4097 | CA | HIS | 522 | 118.634 | 31.715 | 59.176 | 1.00 | 63.52 |
| 5 | 4098 | CB | HIS | 522 | 119.500 | 32.851 | 59.730 | 1.00 | 73.38 |
| | 4099 | CG | HIS | 522 | 120.971 | 32.581 | 59.659 | 1.00 | 84.65 |
| | 4100 | CD2 | HIS | 522 | 122.020 | 33.405 | 59.421 | 1.00 | 85.52 |
| | 4101 | ND1 | HIS | 522 | 121.508 | 31.324 | 59.848 | 1.00 | 87.86 |
| | 4102 | CE1 | HIS | 522 | 122.822 | 31.386 | 59.729 | 1.00 | 88.53 |
| 10 | 4103 | NE2 | HIS | 522 | 123.158 | 32.637 | 59.470 | 1.00 | 88.81 |
| | 4104 | C | HIS | 522 | 117.159 | 31.977 | 59.482 | 1.00 | 63.87 |
| | 4105 | O | HIS | 522 | 116.816 | 32.500 | 60.546 | 1.00 | 62.90 |
| | 4106 | N | ASN | 523 | 116.300 | 31.606 | 58.534 | 1.00 | 61.66 |
| | 4107 | CA | ASN | 523 | 114.850 | 31.771 | 58.635 | 1.00 | 60.61 |
| 15 | 4108 | CB | ASN | 523 | 114.273 | 30.822 | 59.691 | 1.00 | 60.04 |
| | 4109 | CG | ASN | 523 | 112.807 | 30.509 | 59.453 | 1.00 | 59.80 |
| | 4110 | OD1 | ASN | 523 | 112.388 | 30.266 | 58.319 | 1.00 | 62.26 |
| | 4111 | ND2 | ASN | 523 | 112.021 | 30.510 | 60.522 | 1.00 | 59.58 |
| | 4112 | C | ASN | 523 | 114.434 | 33.220 | 58.910 | 1.00 | 60.32 |
| 20 | 4113 | O | ASN | 523 | 113.481 | 33.486 | 59.649 | 1.00 | 55.47 |
| | 4114 | N | LEU | 524 | 115.162 | 34.149 | 58.295 | 1.00 | 61.14 |
| | 4115 | CA | LEU | 524 | 114.905 | 35.577 | 58.436 | 1.00 | 59.79 |
| | 4116 | CB | LEU | 524 | 115.935 | 36.223 | 59.371 | 1.00 | 62.62 |
| | 4117 | CG | LEU | 524 | 115.945 | 35.764 | 60.835 | 1.00 | 65.24 |
| 25 | 4118 | CD1 | LEU | 524 | 117.147 | 36.347 | 61.567 | 1.00 | 65.21 |
| | 4119 | CD2 | LEU | 524 | 114.642 | 36.163 | 61.521 | 1.00 | 62.62 |
| | 4120 | C | LEU | 524 | 114.966 | 36.235 | 57.065 | 1.00 | 59.79 |
| | 4121 | O | LEU | 524 | 115.721 | 35.800 | 56.189 | 1.00 | 56.91 |
| | 4122 | N | ASP | 525 | 114.156 | 37.274 | 56.882 | 1.00 | 62.76 |
| 30 | 4123 | CA | ASP | 525 | 114.100 | 38.006 | 55.620 | 1.00 | 59.59 |
| | 4124 | CB | ASP | 525 | 112.987 | 39.055 | 55.670 | 1.00 | 58.10 |
| | 4125 | CG | ASP | 525 | 112.641 | 39.608 | 54.302 | 1.00 | 60.27 |
| | 4126 | OD1 | ASP | 525 | 113.331 | 39.276 | 53.315 | 1.00 | 58.07 |
| | 4127 | OD2 | ASP | 525 | 111.660 | 40.374 | 54.210 | 1.00 | 64.63 |
| 35 | 4128 | C | ASP | 525 | 115.448 | 38.668 | 55.332 | 1.00 | 59.32 |
| | 4129 | O | ASP | 525 | 115.753 | 39.740 | 55.854 | 1.00 | 63.36 |
| | 4130 | N | GLY | 526 | 116.239 | 38.028 | 54.478 | 1.00 | 58.65 |
| | 4131 | CA | GLY | 526 | 117.557 | 38.536 | 54.149 | 1.00 | 55.69 |
| | 4132 | C | GLY | 526 | 117.641 | 39.797 | 53.316 | 1.00 | 53.62 |
| 40 | 4133 | O | GLY | 526 | 118.648 | 40.502 | 53.372 | 1.00 | 60.05 |
| | 4134 | N | TYR | 527 | 116.607 | 40.085 | 52.534 | 1.00 | 51.88 |
| | 4135 | CA | TYR | 527 | 116.617 | 41.285 | 51.702 | 1.00 | 55.73 |
| | 4136 | CB | TYR | 527 | 115.648 | 41.119 | 50.545 | 1.00 | 55.31 |
| | 4137 | CG | TYR | 527 | 115.562 | 42.295 | 49.598 | 1.00 | 57.45 |
| 45 | 4138 | CD1 | TYR | 527 | 116.330 | 42.336 | 48.433 | 1.00 | 58.75 |
| | 4139 | CE1 | TYR | 527 | 116.193 | 43.375 | 47.518 | 1.00 | 59.49 |
| | 4140 | CD2 | TYR | 527 | 114.656 | 43.332 | 49.824 | 1.00 | 58.17 |
| | 4141 | CE2 | TYR | 527 | 114.511 | 44.373 | 48.917 | 1.00 | 56.67 |
| | 4142 | CZ | TYR | 527 | 115.282 | 44.388 | 47.767 | 1.00 | 57.63 |
| 50 | 4143 | OH | TYR | 527 | 115.159 | 45.420 | 46.868 | 1.00 | 55.43 |

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|----|------|-----|-----|-----|---------|--------|--------|------|--------|
| | 4144 | C | TYR | 527 | 116.266 | 42.524 | 52.517 | 1.00 | 58.54 |
| | 4145 | O | TYR | 527 | 116.862 | 43.593 | 52.342 | 1.00 | 58.64 |
| | 4146 | N | THR | 528 | 115.271 | 42.383 | 53.386 | 1.00 | 59.24 |
| | 4147 | CA | THR | 528 | 114.855 | 43.486 | 54.238 | 1.00 | 59.20 |
| 5 | 4148 | CB | THR | 528 | 113.447 | 43.253 | 54.836 | 1.00 | 54.20 |
| | 4149 | OG1 | THR | 528 | 112.504 | 43.053 | 53.776 | 1.00 | 47.41 |
| | 4150 | CG2 | THR | 528 | 113.010 | 44.458 | 55.655 | 1.00 | 54.59 |
| | 4151 | C | THR | 528 | 115.887 | 43.653 | 55.356 | 1.00 | 60.28 |
| | 4152 | O | THR | 528 | 116.168 | 44.773 | 55.787 | 1.00 | 63.64 |
| 10 | 4153 | N | HIS | 529 | 116.464 | 42.533 | 55.792 | 1.00 | 61.45 |
| | 4154 | CA | HIS | 529 | 117.484 | 42.512 | 56.842 | 1.00 | 66.52 |
| | 4155 | CB | HIS | 529 | 116.984 | 41.721 | 58.060 | 1.00 | 66.73 |
| | 4156 | CG | HIS | 529 | 115.652 | 42.169 | 58.576 | 1.00 | 71.41 |
| | 4157 | CD2 | HIS | 529 | 115.119 | 43.407 | 58.721 | 1.00 | 72.13 |
| 15 | 4158 | ND1 | HIS | 529 | 114.688 | 41.286 | 59.010 | 1.00 | 74.46 |
| | 4159 | CE1 | HIS | 529 | 113.618 | 41.958 | 59.398 | 1.00 | 72.55 |
| | 4160 | NE2 | HIS | 529 | 113.856 | 43.248 | 59.232 | 1.00 | 70.77 |
| | 4161 | C | HIS | 529 | 118.743 | 41.844 | 56.273 | 1.00 | 66.01 |
| | 4162 | O | HIS | 529 | 119.005 | 40.665 | 56.528 | 1.00 | 68.54 |
| 20 | 4163 | N | PRO | 530 | 119.540 | 42.598 | 55.492 | 1.00 | 63.94 |
| | 4164 | CD | PRO | 530 | 119.254 | 43.981 | 55.082 | 1.00 | 59.34 |
| | 4165 | CA | PRO | 530 | 120.778 | 42.128 | 54.856 | 1.00 | 66.66 |
| | 4166 | CB | PRO | 530 | 121.137 | 43.284 | 53.914 | 1.00 | 62.98 |
| | 4167 | CG | PRO | 530 | 119.837 | 44.009 | 53.711 | 1.00 | 59.02 |
| 25 | 4168 | C | PRO | 530 | 121.952 | 41.819 | 55.784 | 1.00 | 70.87 |
| | 4169 | O | PRO | 530 | 122.567 | 40.757 | 55.682 | 1.00 | 73.58 |
| | 4170 | N | GLU | 531 | 122.248 | 42.762 | 56.676 | 1.00 | 73.21 |
| | 4171 | CA | GLU | 531 | 123.365 | 42.683 | 57.621 | 1.00 | 73.20 |
| | 4172 | CB | GLU | 531 | 123.107 | 43.597 | 58.822 | 1.00 | 75.84 |
| 30 | 4173 | CG | GLU | 531 | 124.335 | 43.811 | 59.703 | 1.00 | 84.33 |
| | 4174 | CD | GLU | 531 | 124.108 | 44.832 | 60.799 | 1.00 | 87.41 |
| | 4175 | OE1 | GLU | 531 | 123.904 | 46.021 | 60.474 | 1.00 | 95.89 |
| | 4176 | OE2 | GLU | 531 | 124.142 | 44.446 | 61.986 | 1.00 | 83.48 |
| | 4177 | C | GLU | 531 | 123.843 | 41.312 | 58.106 | 1.00 | 71.16 |
| 35 | 4178 | O | GLU | 531 | 125.042 | 41.026 | 58.066 | 1.00 | 69.83 |
| | 4179 | N | GLU | 532 | 122.923 | 40.470 | 58.563 | 1.00 | 69.84 |
| | 4180 | CA | GLU | 532 | 123.299 | 39.151 | 59.064 | 1.00 | 69.95 |
| | 4181 | CB | GLU | 532 | 122.239 | 38.621 | 60.028 | 1.00 | 76.12 |
| | 4182 | CG | GLU | 532 | 122.200 | 39.350 | 61.360 | 1.00 | 90.10 |
| 40 | 4183 | CD | GLU | 532 | 121.231 | 38.719 | 62.343 | 1.00 | 99.66 |
| | 4184 | OE1 | GLU | 532 | 121.294 | 37.485 | 62.540 | 1.00 | 100.00 |
| | 4185 | OE2 | GLU | 532 | 120.407 | 39.460 | 62.922 | 1.00 | 100.00 |
| | 4186 | C | GLU | 532 | 123.601 | 38.095 | 58.006 | 1.00 | 65.98 |
| | 4187 | O | GLU | 532 | 124.484 | 37.257 | 58.202 | 1.00 | 65.68 |
| 45 | 4188 | N | VAL | 533 | 122.878 | 38.136 | 56.891 | 1.00 | 60.94 |
| | 4189 | CA | VAL | 533 | 123.071 | 37.152 | 55.829 | 1.00 | 51.25 |
| | 4190 | CB | VAL | 533 | 121.727 | 36.491 | 55.419 | 1.00 | 57.84 |
| | 4191 | CG1 | VAL | 533 | 121.983 | 35.305 | 54.492 | 1.00 | 49.96 |
| | 4192 | CG2 | VAL | 533 | 120.942 | 36.054 | 56.655 | 1.00 | 58.45 |
| 50 | 4193 | C | VAL | 533 | 123.741 | 37.704 | 54.574 | 1.00 | 44.33 |

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|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 4194 | O | VAL | 533 | 124.834 | 37.270 | 54.208 | 1.00 | 42.16 |
| | 4195 | N | LEU | 534 | 123.085 | 38.662 | 53.925 | 1.00 | 37.63 |
| | 4196 | CA | LEU | 534 | 123.590 | 39.249 | 52.687 | 1.00 | 27.92 |
| | 4197 | CB | LEU | 534 | 122.499 | 40.068 | 52.002 | 1.00 | 24.48 |
| 5 | 4198 | CG | LEU | 534 | 121.258 | 39.299 | 51.554 | 1.00 | 25.70 |
| | 4199 | CD1 | LEU | 534 | 120.395 | 40.207 | 50.696 | 1.00 | 29.78 |
| | 4200 | CD2 | LEU | 534 | 121.657 | 38.064 | 50.769 | 1.00 | 19.34 |
| | 4201 | C | LEU | 534 | 124.864 | 40.076 | 52.770 | 1.00 | 29.24 |
| | 4202 | O | LEU | 534 | 125.661 | 40.069 | 51.834 | 1.00 | 31.85 |
| 10 | 4203 | N | LYS | 535 | 125.053 | 40.793 | 53.875 | 1.00 | 30.62 |
| | 4204 | CA | LYS | 535 | 126.239 | 41.632 | 54.047 | 1.00 | 30.24 |
| | 4205 | CB | LYS | 535 | 126.251 | 42.276 | 55.439 | 1.00 | 33.69 |
| | 4206 | CG | LYS | 535 | 127.412 | 43.232 | 55.692 | 1.00 | 38.92 |
| | 4207 | CD | LYS | 535 | 127.429 | 43.699 | 57.142 | 1.00 | 43.85 |
| 15 | 4208 | CE | LYS | 535 | 128.605 | 44.617 | 57.425 | 1.00 | 46.39 |
| | 4209 | NZ | LYS | 535 | 128.657 | 45.016 | 58.861 | 1.00 | 46.21 |
| | 4210 | C | LYS | 535 | 127.548 | 40.881 | 53.784 | 1.00 | 30.84 |
| | 4211 | O | LYS | 535 | 128.328 | 41.286 | 52.918 | 1.00 | 28.96 |
| | 4212 | N | PRO | 536 | 127.790 | 39.759 | 54.495 | 1.00 | 26.98 |
| 20 | 4213 | CD | PRO | 536 | 126.965 | 39.148 | 55.554 | 1.00 | 30.04 |
| | 4214 | CA | PRO | 536 | 129.018 | 38.982 | 54.302 | 1.00 | 22.09 |
| | 4215 | CB | PRO | 536 | 128.796 | 37.772 | 55.206 | 1.00 | 22.33 |
| | 4216 | CG | PRO | 536 | 127.975 | 38.330 | 56.312 | 1.00 | 25.59 |
| | 4217 | C | PRO | 536 | 129.213 | 38.551 | 52.853 | 1.00 | 23.63 |
| 25 | 4218 | O | PRO | 536 | 130.313 | 38.660 | 52.315 | 1.00 | 34.37 |
| | 4219 | N | HIS | 537 | 128.137 | 38.082 | 52.226 | 1.00 | 21.41 |
| | 4220 | CA | HIS | 537 | 128.180 | 37.635 | 50.836 | 1.00 | 16.74 |
| | 4221 | CB | HIS | 537 | 126.812 | 37.108 | 50.393 | 1.00 | 17.36 |
| | 4222 | CG | HIS | 537 | 126.392 | 35.849 | 51.086 | 1.00 | 26.82 |
| 30 | 4223 | CD2 | HIS | 537 | 125.171 | 35.406 | 51.467 | 1.00 | 19.54 |
| | 4224 | ND1 | HIS | 537 | 127.289 | 34.872 | 51.465 | 1.00 | 20.86 |
| | 4225 | CE1 | HIS | 537 | 126.638 | 33.883 | 52.050 | 1.00 | 21.91 |
| | 4226 | NE2 | HIS | 537 | 125.351 | 34.182 | 52.064 | 1.00 | 18.99 |
| | 4227 | C | HIS | 537 | 128.611 | 38.757 | 49.910 | 1.00 | 19.57 |
| 35 | 4228 | O | HIS | 537 | 129.477 | 38.569 | 49.060 | 1.00 | 24.18 |
| | 4229 | N | ILE | 538 | 128.003 | 39.927 | 50.091 | 1.00 | 25.84 |
| | 4230 | CA | ILE | 538 | 128.307 | 41.101 | 49.279 | 1.00 | 25.72 |
| | 4231 | CB | ILE | 538 | 127.331 | 42.262 | 49.600 | 1.00 | 25.90 |
| | 4232 | CG2 | ILE | 538 | 127.739 | 43.536 | 48.856 | 1.00 | 21.31 |
| 40 | 4233 | CG1 | ILE | 538 | 125.905 | 41.849 | 49.219 | 1.00 | 14.44 |
| | 4234 | CD1 | ILE | 538 | 124.847 | 42.872 | 49.559 | 1.00 | 19.77 |
| | 4235 | C | ILE | 538 | 129.760 | 41.545 | 49.467 | 1.00 | 24.83 |
| | 4236 | O | ILE | 538 | 130.419 | 41.957 | 48.510 | 1.00 | 17.63 |
| | 4237 | N | ILE | 539 | 130.255 | 41.440 | 50.698 | 1.00 | 19.39 |
| 45 | 4238 | CA | ILE | 539 | 131.632 | 41.809 | 51.002 | 1.00 | 25.84 |
| | 4239 | CB | ILE | 539 | 131.882 | 41.864 | 52.532 | 1.00 | 31.48 |
| | 4240 | CG2 | ILE | 539 | 133.375 | 41.923 | 52.835 | 1.00 | 28.38 |
| | 4241 | CG1 | ILE | 539 | 131.172 | 43.078 | 53.137 | 1.00 | 26.00 |
| | 4242 | CD1 | ILE | 539 | 131.381 | 43.224 | 54.633 | 1.00 | 28.00 |
| 50 | 4243 | C | ILE | 539 | 132.598 | 40.819 | 50.355 | 1.00 | 24.71 |

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|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 4244 | O | ILE | 539 | 133.587 | 41.218 | 49.742 | 1.00 | 30.21 |
| | 4245 | N | ASN | 540 | 132.286 | 39.531 | 50.461 | 1.00 | 22.80 |
| | 4246 | CA | ASN | 540 | 133.132 | 38.487 | 49.892 | 1.00 | 16.68 |
| | 4247 | CB | ASN | 540 | 132.802 | 37.135 | 50.525 | 1.00 | 17.40 |
| 5 | 4248 | CG | ASN | 540 | 133.009 | 37.126 | 52.032 | 1.00 | 26.52 |
| | 4249 | OD1 | ASN | 540 | 132.357 | 36.371 | 52.755 | 1.00 | 29.84 |
| | 4250 | ND2 | ASN | 540 | 133.918 | 37.969 | 52.511 | 1.00 | 25.48 |
| | 4251 | C | ASN | 540 | 133.039 | 38.386 | 48.371 | 1.00 | 16.85 |
| | 4252 | O | ASN | 540 | 133.933 | 37.832 | 47.733 | 1.00 | 18.60 |
| 10 | 4253 | N | LEU | 541 | 131.979 | 38.944 | 47.789 | 1.00 | 16.65 |
| | 4254 | CA | LEU | 541 | 131.791 | 38.889 | 46.340 | 1.00 | 19.54 |
| | 4255 | CB | LEU | 541 | 130.393 | 38.360 | 46.001 | 1.00 | 16.13 |
| | 4256 | CG | LEU | 541 | 130.003 | 36.954 | 46.463 | 1.00 | 16.63 |
| | 4257 | CD1 | LEU | 541 | 128.588 | 36.662 | 46.017 | 1.00 | 9.71 |
| 15 | 4258 | CD2 | LEU | 541 | 130.960 | 35.919 | 45.901 | 1.00 | 11.40 |
| | 4259 | C | LEU | 541 | 132.016 | 40.198 | 45.585 | 1.00 | 22.24 |
| | 4260 | O | LEU | 541 | 132.528 | 40.186 | 44.464 | 1.00 | 22.51 |
| | 4261 | N | LEU | 542 | 131.642 | 41.321 | 46.192 | 1.00 | 23.86 |
| | 4262 | CA | LEU | 542 | 131.774 | 42.619 | 45.531 | 1.00 | 27.26 |
| 20 | 4263 | CB | LEU | 542 | 130.392 | 43.266 | 45.412 | 1.00 | 30.85 |
| | 4264 | CG | LEU | 542 | 129.374 | 42.454 | 44.608 | 1.00 | 33.63 |
| | 4265 | CD1 | LEU | 542 | 127.960 | 42.968 | 44.844 | 1.00 | 33.98 |
| | 4266 | CD2 | LEU | 542 | 129.741 | 42.505 | 43.137 | 1.00 | 30.60 |
| | 4267 | C | LEU | 542 | 132.770 | 43.621 | 46.124 | 1.00 | 30.35 |
| 25 | 4268 | O | LEU | 542 | 133.102 | 44.615 | 45.474 | 1.00 | 32.15 |
| | 4269 | N | VAL | 543 | 133.234 | 43.373 | 47.348 | 1.00 | 20.35 |
| | 4270 | CA | VAL | 543 | 134.192 | 44.263 | 48.008 | 1.00 | 17.15 |
| | 4271 | CB | VAL | 543 | 133.758 | 44.564 | 49.466 | 1.00 | 22.13 |
| | 4272 | CG1 | VAL | 543 | 134.761 | 45.485 | 50.147 | 1.00 | 18.99 |
| 30 | 4273 | CG2 | VAL | 543 | 132.369 | 45.184 | 49.485 | 1.00 | 25.56 |
| | 4274 | C | VAL | 543 | 135.608 | 43.670 | 48.012 | 1.00 | 20.12 |
| | 4275 | O | VAL | 543 | 136.484 | 44.106 | 47.259 | 1.00 | 14.30 |
| | 4276 | N | ASP | 544 | 135.813 | 42.667 | 48.860 | 1.00 | 22.55 |
| | 4277 | CA | ASP | 544 | 137.102 | 41.999 | 48.992 | 1.00 | 17.64 |
| 35 | 4278 | CB | ASP | 544 | 137.183 | 41.246 | 50.326 | 1.00 | 10.56 |
| | 4279 | CG | ASP | 544 | 137.103 | 42.164 | 51.532 | 1.00 | 22.81 |
| | 4280 | OD1 | ASP | 544 | 136.839 | 41.648 | 52.639 | 1.00 | 23.90 |
| | 4281 | OD2 | ASP | 544 | 137.313 | 43.390 | 51.385 | 1.00 | 33.46 |
| | 4282 | C | ASP | 544 | 137.389 | 41.018 | 47.868 | 1.00 | 18.71 |
| 40 | 4283 | O | ASP | 544 | 136.548 | 40.191 | 47.517 | 1.00 | 20.02 |
| | 4284 | N | SER | 545 | 138.590 | 41.116 | 47.310 | 1.00 | 23.60 |
| | 4285 | CA | SER | 545 | 139.022 | 40.215 | 46.253 | 1.00 | 27.74 |
| | 4286 | CB | SER | 545 | 139.900 | 40.957 | 45.243 | 1.00 | 27.70 |
| | 4287 | OG | SER | 545 | 141.043 | 41.512 | 45.871 | 1.00 | 32.50 |
| 45 | 4288 | C | SER | 545 | 139.823 | 39.098 | 46.920 | 1.00 | 31.23 |
| | 4289 | O | SER | 545 | 140.409 | 39.303 | 47.987 | 1.00 | 32.16 |
| | 4290 | N | ILE | 546 | 139.816 | 37.913 | 46.317 | 1.00 | 30.36 |
| | 4291 | CA | ILE | 546 | 140.558 | 36.780 | 46.863 | 1.00 | 33.30 |
| | 4292 | CB | ILE | 546 | 140.281 | 35.475 | 46.072 | 1.00 | 33.46 |
| 50 | 4293 | CG2 | ILE | 546 | 141.051 | 34.310 | 46.686 | 1.00 | 27.25 |

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|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 4294 | CG1 | ILE | 546 | 138.783 | 35.165 | 46.072 | 1.00 | 27.20 |
| | 4295 | CD1 | ILE | 546 | 138.418 | 33.915 | 45.319 | 1.00 | 23.76 |
| | 4296 | C | ILE | 546 | 142.041 | 37.113 | 46.765 | 1.00 | 35.94 |
| | 4297 | O | ILE | 546 | 142.559 | 37.332 | 45.668 | 1.00 | 34.27 |
| 5 | 4298 | N | LYS | 547 | 142.708 | 37.200 | 47.913 | 1.00 | 37.96 |
| | 4299 | CA | LYS | 547 | 144.131 | 37.518 | 47.929 | 1.00 | 45.36 |
| | 4300 | CB | LYS | 547 | 144.581 | 37.989 | 49.318 | 1.00 | 53.18 |
| | 4301 | CG | LYS | 547 | 144.193 | 37.086 | 50.476 | 1.00 | 62.91 |
| | 4302 | CD | LYS | 547 | 144.627 | 37.709 | 51.796 | 1.00 | 73.57 |
| 10 | 4303 | CE | LYS | 547 | 144.241 | 36.839 | 52.982 | 1.00 | 81.58 |
| | 4304 | NZ | LYS | 547 | 144.683 | 37.440 | 54.274 | 1.00 | 85.95 |
| | 4305 | C | LYS | 547 | 144.986 | 36.359 | 47.425 | 1.00 | 43.05 |
| | 4306 | O | LYS | 547 | 144.897 | 35.236 | 47.921 | 1.00 | 34.62 |
| | 4307 | N | ILE | 548 | 145.778 | 36.648 | 46.396 | 1.00 | 45.90 |
| 15 | 4308 | CA | ILE | 548 | 146.656 | 35.666 | 45.771 | 1.00 | 45.52 |
| | 4309 | CB | ILE | 548 | 147.148 | 36.170 | 44.394 | 1.00 | 41.81 |
| | 4310 | CG2 | ILE | 548 | 147.927 | 35.073 | 43.679 | 1.00 | 45.55 |
| | 4311 | CG1 | ILE | 548 | 145.951 | 36.603 | 43.540 | 1.00 | 39.14 |
| | 4312 | CD1 | ILE | 548 | 146.327 | 37.269 | 42.238 | 1.00 | 45.90 |
| 20 | 4313 | C | ILE | 548 | 147.856 | 35.342 | 46.659 | 1.00 | 48.55 |
| | 4314 | OT1 | ILE | 548 | 148.019 | 34.153 | 47.005 | 1.00 | 46.58 |
| | 4315 | OT2 | ILE | 548 | 148.606 | 36.278 | 47.012 | 1.00 | 59.90 |
| | 4316 | OH2 | WAT | 601 | 109.544 | 21.898 | 33.684 | 1.00 | 2.00 |
| | 4317 | OH2 | WAT | 602 | 132.108 | 38.577 | 42.342 | 1.00 | 3.74 |
| 25 | 4318 | OH2 | WAT | 603 | 121.652 | 22.556 | 52.348 | 1.00 | 5.90 |
| | 4319 | OH2 | WAT | 604 | 136.076 | 10.222 | 44.594 | 1.00 | 31.07 |
| | 4320 | OH2 | WAT | 605 | 131.497 | 21.852 | 51.678 | 1.00 | 7.22 |
| | 4321 | OH2 | WAT | 606 | 128.656 | 14.200 | 45.316 | 1.00 | 17.90 |
| | 4322 | OH2 | WAT | 607 | 124.677 | 19.198 | 47.081 | 1.00 | 15.60 |
| 30 | 4323 | OH2 | WAT | 608 | 125.455 | 29.812 | 49.014 | 1.00 | 8.48 |
| | 4324 | OH2 | WAT | 609 | 105.474 | 36.871 | 39.547 | 1.00 | 9.05 |
| | 4325 | OH2 | WAT | 610 | 133.536 | 36.915 | 40.513 | 1.00 | 19.37 |
| | 4326 | OH2 | WAT | 611 | 126.730 | 22.375 | 41.980 | 1.00 | 17.96 |
| | 4327 | OH2 | WAT | 612 | 133.379 | 23.457 | 50.388 | 1.00 | 16.43 |
| 35 | 4328 | OH2 | WAT | 613 | 136.836 | 31.698 | 39.273 | 1.00 | 23.48 |
| | 4329 | OH2 | WAT | 614 | 130.615 | 20.278 | 41.368 | 1.00 | 11.16 |
| | 4330 | OH2 | WAT | 615 | 127.633 | 29.682 | 51.807 | 1.00 | 16.49 |
| | 4331 | OH2 | WAT | 616 | 100.533 | 31.281 | 26.832 | 1.00 | 34.28 |
| | 4332 | OH2 | WAT | 617 | 121.692 | 21.167 | 34.150 | 1.00 | 25.91 |
| 40 | 4333 | OH2 | WAT | 618 | 131.226 | 32.257 | 50.439 | 1.00 | 34.81 |
| | 4334 | OH2 | WAT | 619 | 88.365 | 35.120 | 57.147 | 1.00 | 33.73 |
| | 4335 | OH2 | WAT | 620 | 118.147 | 18.317 | 26.341 | 1.00 | 21.70 |
| | 4336 | OH2 | WAT | 621 | 113.190 | 8.087 | 35.703 | 1.00 | 36.62 |
| | 4337 | OH2 | WAT | 622 | 125.312 | 30.072 | 37.791 | 1.00 | 30.00 |
| 45 | 4338 | OH2 | WAT | 623 | 92.432 | 24.852 | 50.099 | 1.00 | 25.65 |
| | 4339 | OH2 | WAT | 624 | 108.974 | 15.165 | 49.075 | 1.00 | 21.10 |
| | 4340 | OH2 | WAT | 625 | 135.431 | 14.884 | 45.393 | 1.00 | 46.74 |
| | 4341 | OH2 | WAT | 626 | 115.012 | 4.805 | 43.826 | 1.00 | 30.43 |
| | 4342 | OH2 | WAT | 627 | 88.415 | 44.463 | 58.820 | 1.00 | 30.86 |
| 50 | 4343 | OH2 | WAT | 628 | 125.976 | 25.755 | 43.265 | 1.00 | 27.75 |

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|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 4344 | OH2 | WAT | 629 | 117.921 | 5.153 | 51.682 | 1.00 | 34.87 |
| | 4345 | OH2 | WAT | 630 | 91.157 | 43.104 | 44.532 | 1.00 | 27.09 |
| | 4346 | OH2 | WAT | 631 | 114.902 | 63.428 | 42.828 | 1.00 | 30.49 |
| | 4347 | OH2 | WAT | 632 | 99.150 | 43.135 | 52.476 | 1.00 | 17.32 |
| 5 | 4348 | OH2 | WAT | 633 | 116.849 | 14.286 | 50.256 | 1.00 | 20.41 |
| | 4349 | OH2 | WAT | 634 | 136.092 | 41.410 | 33.663 | 1.00 | 26.72 |
| | 4350 | OH2 | WAT | 635 | 104.683 | 23.377 | 25.808 | 1.00 | 36.55 |
| | 4351 | OH2 | WAT | 636 | 133.163 | 25.808 | 57.616 | 1.00 | 29.75 |
| | 4352 | OH2 | WAT | 637 | 130.650 | 30.337 | 40.643 | 1.00 | 11.08 |
| 10 | 4353 | OH2 | WAT | 638 | 141.018 | 40.362 | 50.563 | 1.00 | 27.14 |
| | 4354 | OH2 | WAT | 639 | 126.744 | 19.348 | 30.510 | 1.00 | 20.69 |
| | 4355 | OH2 | WAT | 640 | 99.257 | 26.859 | 66.394 | 1.00 | 32.76 |
| | 4356 | OH2 | WAT | 641 | 107.042 | 13.044 | 38.812 | 1.00 | 37.53 |
| | 4357 | OH2 | WAT | 642 | 111.411 | 17.702 | 31.576 | 1.00 | 25.63 |
| 15 | 4358 | OH2 | WAT | 643 | 136.247 | 16.841 | 49.081 | 1.00 | 26.74 |
| | 4359 | OH2 | WAT | 644 | 130.107 | 34.877 | 51.432 | 1.00 | 22.05 |
| | 4360 | OH2 | WAT | 645 | 131.572 | 27.845 | 36.507 | 1.00 | 33.61 |
| | 4361 | OH2 | WAT | 646 | 139.273 | 18.921 | 51.935 | 1.00 | 18.69 |
| | 4362 | OH2 | WAT | 647 | 102.180 | 34.258 | 26.188 | 1.00 | 38.28 |
| 20 | 4363 | OH2 | WAT | 648 | 123.655 | 36.667 | 26.709 | 1.00 | 23.51 |
| | 4364 | OH2 | WAT | 649 | 126.661 | 35.233 | 55.363 | 1.00 | 32.41 |
| | 4365 | OH2 | WAT | 650 | 106.153 | 21.764 | 42.249 | 1.00 | 20.34 |
| | 4366 | OH2 | WAT | 651 | 135.834 | 34.833 | 30.691 | 1.00 | 52.17 |
| | 4367 | OH2 | WAT | 652 | 103.106 | 38.892 | 25.426 | 1.00 | 26.00 |
| 25 | 4368 | OH2 | WAT | 653 | 140.880 | 35.431 | 50.226 | 1.00 | 26.45 |
| | 4369 | OH2 | WAT | 654 | 112.327 | 13.971 | 50.722 | 1.00 | 46.47 |
| | 4370 | OH2 | WAT | 655 | 142.876 | 32.708 | 49.617 | 1.00 | 38.19 |
| | 4371 | OH2 | WAT | 656 | 136.448 | 11.686 | 63.277 | 1.00 | 31.93 |
| | 4372 | OH2 | WAT | 657 | 128.522 | 28.120 | 35.575 | 1.00 | 25.65 |
| 30 | 4373 | OH2 | WAT | 658 | 124.837 | 30.666 | 35.131 | 1.00 | 22.56 |
| | 4374 | OH2 | WAT | 659 | 130.833 | 34.205 | 29.481 | 1.00 | 42.51 |
| | 4375 | OH2 | WAT | 660 | 112.306 | 35.037 | 18.431 | 1.00 | 22.73 |
| | 4376 | OH2 | WAT | 661 | 121.695 | 49.220 | 48.983 | 1.00 | 34.50 |
| | 4377 | OH2 | WAT | 662 | 134.850 | 24.747 | 24.896 | 1.00 | 61.06 |
| 35 | 4378 | OH2 | WAT | 663 | 120.492 | 22.780 | 56.510 | 1.00 | 33.74 |
| | 4379 | OH2 | WAT | 664 | 145.265 | 41.024 | 28.023 | 1.00 | 26.03 |
| | 4380 | OH2 | WAT | 665 | 92.325 | 61.829 | 41.100 | 1.00 | 63.45 |
| | 4381 | OH2 | WAT | 666 | 122.583 | 51.518 | 33.284 | 1.00 | 48.58 |
| | 4382 | OH2 | WAT | 667 | 134.126 | 51.766 | 45.296 | 1.00 | 19.94 |
| 40 | 4383 | OH2 | WAT | 668 | 99.217 | 28.001 | 33.331 | 1.00 | 36.10 |
| | 4384 | OH2 | WAT | 669 | 116.117 | 48.969 | 45.889 | 1.00 | 27.24 |
| | 4385 | OH2 | WAT | 670 | 90.118 | 37.836 | 45.821 | 1.00 | 21.42 |
| | 4386 | OH2 | WAT | 671 | 140.530 | 43.280 | 48.000 | 1.00 | 25.45 |
| | 4387 | OH2 | WAT | 672 | 91.812 | 21.421 | 53.465 | 1.00 | 25.28 |
| 45 | 4388 | OH2 | WAT | 673 | 133.156 | 2.402 | 49.442 | 1.00 | 44.64 |
| | 4389 | OH2 | WAT | 674 | 124.710 | 30.183 | 52.286 | 1.00 | 27.01 |
| | 4390 | OH2 | WAT | 675 | 108.046 | 22.156 | 30.804 | 1.00 | 29.23 |
| | 4391 | OH2 | WAT | 676 | 141.812 | 18.051 | 53.703 | 1.00 | 33.60 |
| | 4392 | OH2 | WAT | 677 | 122.438 | 4.780 | 34.061 | 1.00 | 22.75 |
| 50 | 4393 | OH2 | WAT | 678 | 106.890 | 50.310 | 27.843 | 1.00 | 27.59 |

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|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 4394 | OH2 | WAT | 679 | 99.813 | 44.123 | 49.703 | 1.00 | 35.15 |
| | 4395 | OH2 | WAT | 680 | 114.424 | 25.540 | 53.859 | 1.00 | 59.82 |
| | 4396 | OH2 | WAT | 681 | 120.122 | 17.036 | 61.627 | 1.00 | 33.13 |
| | 4397 | OH2 | WAT | 682 | 123.491 | 39.726 | 28.595 | 1.00 | 39.84 |
| 5 | 4398 | OH2 | WAT | 683 | 120.197 | 47.611 | 55.219 | 1.00 | 29.64 |
| | 4399 | OH2 | WAT | 684 | 103.132 | 41.401 | 52.472 | 1.00 | 31.67 |
| | 4400 | OH2 | WAT | 685 | 95.409 | 27.232 | 43.768 | 1.00 | 40.36 |
| | 4401 | OH2 | WAT | 686 | 93.494 | 47.869 | 47.074 | 1.00 | 41.27 |
| | 4402 | OH2 | WAT | 687 | 101.201 | 66.857 | 39.062 | 1.00 | 78.46 |
| 10 | 4403 | OH2 | WAT | 688 | 117.640 | 29.026 | 61.987 | 1.00 | 47.48 |
| | 4404 | OH2 | WAT | 689 | 125.779 | 23.773 | 30.324 | 1.00 | 37.41 |
| | 4405 | OH2 | WAT | 690 | 118.394 | 14.351 | 39.712 | 1.00 | 8.48 |
| | 4406 | OH2 | WAT | 691 | 115.774 | 17.384 | 46.942 | 1.00 | 55.16 |
| | 4407 | OH2 | WAT | 692 | 125.846 | 32.742 | 40.650 | 1.00 | 30.56 |
| 15 | 4408 | OH2 | WAT | 693 | 134.539 | 32.766 | 51.897 | 1.00 | 52.33 |
| | 4409 | OH2 | WAT | 694 | 132.231 | 24.088 | 46.766 | 1.00 | 63.16 |
| | 4410 | OH2 | WAT | 695 | 120.423 | 11.828 | 28.871 | 1.00 | 44.89 |
| | 4411 | OH2 | WAT | 696 | 109.529 | 18.849 | 35.510 | 1.00 | 41.86 |
| | 4412 | OH2 | WAT | 697 | 126.344 | 22.049 | 35.670 | 1.00 | 37.93 |
| 20 | 4413 | OH2 | WAT | 698 | 140.761 | 46.564 | 40.929 | 1.00 | 36.10 |
| | 4414 | OH2 | WAT | 699 | 149.712 | 28.211 | 43.996 | 1.00 | 63.77 |
| | 4415 | OH2 | WAT | 700 | 122.788 | 19.483 | 59.019 | 1.00 | 46.07 |
| | 4416 | OH2 | WAT | 701 | 133.230 | 48.486 | 44.266 | 1.00 | 36.68 |
| | 4417 | OH2 | WAT | 702 | 121.294 | 17.890 | 56.388 | 1.00 | 45.00 |
| 25 | 4418 | OH2 | WAT | 703 | 129.924 | 31.321 | 53.670 | 1.00 | 28.12 |
| | 4419 | OH2 | WAT | 704 | 130.041 | 22.759 | 34.128 | 1.00 | 58.80 |
| | 4420 | OH2 | WAT | 705 | 120.990 | 14.019 | 62.153 | 1.00 | 90.42 |
| | 4421 | OH2 | WAT | 706 | 144.565 | 20.274 | 60.540 | 1.00 | 57.31 |
| | 4422 | OH2 | WAT | 707 | 122.007 | 30.989 | 34.128 | 1.00 | 74.81 |
| 30 | 4423 | OH2 | WAT | 708 | 136.782 | 18.854 | 45.912 | 1.00 | 38.89 |
| | 4424 | OH2 | WAT | 709 | 148.608 | 25.064 | 51.823 | 1.00 | 69.75 |
| | 4425 | OH2 | WAT | 710 | 129.546 | 23.547 | 49.088 | 1.00 | 59.55 |
| | 4426 | OH2 | WAT | 711 | 98.361 | 36.814 | 48.633 | 1.00 | 48.61 |
| | 4427 | OH2 | WAT | 712 | 135.173 | 8.831 | 61.117 | 1.00 | 57.62 |
| 35 | 4428 | OH2 | WAT | 713 | 125.025 | 32.134 | 55.885 | 1.00 | 46.77 |
| | 4429 | OH2 | WAT | 714 | 109.222 | 19.287 | 57.955 | 1.00 | 58.38 |
| | 4430 | OH2 | WAT | 715 | 137.206 | 8.347 | 56.384 | 1.00 | 48.16 |
| | 4431 | OH2 | WAT | 716 | 105.467 | 21.522 | 45.303 | 1.00 | 55.42 |
| | 4432 | OH2 | WAT | 717 | 108.946 | 9.853 | 39.154 | 1.00 | 73.91 |
| 40 | 4433 | OH2 | WAT | 718 | 96.255 | 23.880 | 48.000 | 1.00 | 73.23 |
| | 4434 | OH2 | WAT | 719 | 101.728 | 36.619 | 50.363 | 1.00 | 57.83 |
| | 4435 | OH2 | WAT | 720 | 116.536 | 13.569 | 56.095 | 1.00 | 62.99 |
| | 4436 | OH2 | WAT | 721 | 128.739 | 23.611 | 38.616 | 1.00 | 70.69 |
| | 4437 | OH2 | WAT | 722 | 126.664 | 3.370 | 36.233 | 1.00 | 79.09 |
| 45 | 4438 | OH2 | WAT | 723 | 120.338 | 3.428 | 58.493 | 1.00 | 86.19 |
| | 4439 | OH2 | WAT | 724 | 132.490 | 26.185 | 26.764 | 1.00 | 67.03 |
| | 4440 | OH2 | WAT | 725 | 119.137 | 22.564 | 24.070 | 1.00 | 75.84 |
| | 4441 | OH2 | WAT | 726 | 98.004 | 28.038 | 42.458 | 1.00 | 72.19 |
| | 4442 | OH2 | WAT | 727 | 99.674 | 33.037 | 41.131 | 1.00 | 69.00 |
| 50 | 4443 | OH2 | WAT | 728 | 113.394 | 11.413 | 52.820 | 1.00 | 69.11 |

| | | | | | | | | | |
|----|------|-----|-----|-----|---------|--------|--------|------|--------|
| | 4444 | OH2 | WAT | 729 | 129.629 | 27.848 | 38.891 | 1.00 | 31.80 |
| | 4445 | OH2 | WAT | 730 | 138.391 | 3.193 | 36.697 | 1.00 | 88.33 |
| | 4446 | OH2 | WAT | 731 | 101.751 | 58.675 | 54.521 | 1.00 | 69.41 |
| | 4447 | OH2 | WAT | 732 | 146.260 | 39.908 | 45.702 | 1.00 | 71.98 |
| 5 | 4448 | OH2 | WAT | 733 | 99.632 | 27.238 | 39.217 | 1.00 | 65.15 |
| | 4449 | OH2 | WAT | 734 | 139.029 | 16.241 | 44.768 | 1.00 | 76.36 |
| | 4450 | OH2 | WAT | 735 | 93.410 | 43.367 | 39.907 | 1.00 | 51.51 |
| | 4451 | OH2 | WAT | 736 | 99.833 | 50.411 | 52.960 | 1.00 | 40.10 |
| | 4452 | OH2 | WAT | 737 | 121.822 | 63.145 | 36.945 | 1.00 | 88.71 |
| 10 | 4453 | OH2 | WAT | 738 | 123.231 | 52.111 | 47.051 | 1.00 | 59.41 |
| | 4454 | OH2 | WAT | 739 | 112.095 | 2.568 | 44.854 | 1.00 | 87.55 |
| | 4455 | OH2 | WAT | 740 | 105.823 | 21.588 | 32.912 | 1.00 | 65.78 |
| | 4456 | OH2 | WAT | 741 | 112.121 | 15.677 | 29.574 | 1.00 | 63.57 |
| | 4457 | OH2 | WAT | 742 | 116.006 | 23.098 | 23.234 | 1.00 | 66.58 |
| 15 | 4458 | OH2 | WAT | 743 | 101.396 | 34.063 | 30.976 | 1.00 | 67.78 |
| | 4459 | OH2 | WAT | 744 | 105.307 | 25.170 | 29.199 | 1.00 | 41.04 |
| | 4460 | OH2 | WAT | 745 | 138.659 | 10.582 | 45.837 | 1.00 | 59.51 |
| | 4461 | OH2 | WAT | 746 | 114.904 | 60.800 | 37.648 | 1.00 | 51.77 |
| | 4462 | OH2 | WAT | 747 | 124.430 | 21.295 | 33.036 | 1.00 | 63.60 |
| 20 | 4463 | OH2 | WAT | 748 | 107.809 | 9.528 | 45.664 | 1.00 | 96.91 |
| | 4464 | OH2 | WAT | 749 | 129.675 | 48.310 | 54.546 | 1.00 | 50.35 |
| | 4465 | OH2 | WAT | 750 | 104.938 | 42.943 | 50.401 | 1.00 | 73.99 |
| | 4466 | OH2 | WAT | 751 | 127.598 | 19.431 | 38.063 | 1.00 | 50.28 |
| | 4467 | OH2 | WAT | 752 | 107.804 | 42.960 | 53.690 | 1.00 | 100.00 |
| 25 | 4468 | OH2 | WAT | 753 | 106.996 | 46.067 | 52.208 | 1.00 | 80.89 |
| | 4469 | OH2 | WAT | 754 | 115.697 | 53.285 | 33.391 | 1.00 | 88.83 |
| | 4470 | OH2 | WAT | 755 | 107.557 | 43.929 | 23.164 | 1.00 | 97.00 |
| | 4471 | OH2 | WAT | 756 | 104.503 | 37.526 | 36.972 | 1.00 | 58.13 |
| | 4472 | MG | MG | 757 | 105.326 | 36.717 | 53.406 | 1.00 | 29.00 |
| 30 | 4473 | MG | MG | 758 | 103.375 | 43.256 | 48.861 | 1.00 | 41.96 |
| | 4474 | MG | MG | 759 | 106.905 | 43.906 | 51.594 | 1.00 | 60.57 |
| | 4475 | PA | HPH | 900 | 106.514 | 40.269 | 50.769 | 1.00 | 64.84 |
| | 4476 | O1A | HPH | 900 | 106.467 | 39.079 | 51.657 | 1.00 | 56.34 |
| | 4477 | O2A | HPH | 900 | 106.738 | 41.560 | 51.467 | 1.00 | 62.50 |
| 35 | 4478 | O3A | HPH | 900 | 105.506 | 40.292 | 49.674 | 1.00 | 62.63 |
| | 4479 | O1 | HPH | 900 | 108.952 | 41.335 | 50.186 | 1.00 | 61.96 |
| | 4480 | C1 | HPH | 900 | 108.025 | 40.315 | 49.769 | 1.00 | 64.00 |
| | 4481 | C2 | HPH | 900 | 108.690 | 38.930 | 49.523 | 1.00 | 61.37 |
| | 4482 | C3 | HPH | 900 | 109.069 | 38.562 | 48.285 | 1.00 | 51.27 |
| 40 | 4483 | C4 | HPH | 900 | 109.443 | 37.123 | 48.011 | 1.00 | 49.88 |
| | 4484 | C5 | HPH | 900 | 110.870 | 36.593 | 48.349 | 1.00 | 48.79 |
| | 4485 | C6 | HPH | 900 | 112.049 | 37.566 | 48.069 | 1.00 | 37.71 |
| | 4486 | C7 | HPH | 900 | 112.320 | 38.019 | 46.829 | 1.00 | 34.33 |
| | 4487 | C8 | HPH | 900 | 113.476 | 38.969 | 46.623 | 1.00 | 35.58 |
| 45 | 4488 | C9 | HPH | 900 | 113.227 | 40.333 | 47.247 | 1.00 | 56.66 |
| | 4489 | C10 | HPH | 900 | 113.089 | 40.275 | 48.776 | 1.00 | 68.86 |
| | 4490 | C11 | HPH | 900 | 112.157 | 41.010 | 49.392 | 1.00 | 73.13 |
| | 4491 | C12 | HPH | 900 | 112.037 | 40.934 | 50.893 | 1.00 | 66.86 |
| | 4492 | C15 | HPH | 900 | 108.853 | 39.500 | 47.137 | 1.00 | 54.81 |
| 50 | 4493 | C13 | HPH | 900 | 111.421 | 42.067 | 48.641 | 1.00 | 68.76 |

4494 C14 HPH 900 111.753 37.299 45.656 1.00 41.06

Table 11
Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase
In the Absence of Bound Substrate

| | Atom Type | Atom | Residue | Residue # | X | Y | Z | OCC | B- factor |
|----|--------------|------|---------|--------------|---------|--------|--------|------------|--------------|
| 5 | | | | | | | | | |
| | 1 | N | LEU | 24 | 121.956 | 50.261 | 52.247 | 1.00124.05 | |
| | 2 | CA | LEU | 24 | 122.946 | 50.852 | 53.202 | 1.00125.60 | |
| 10 | 3 | C | LEU | 24 | 124.286 | 50.797 | 52.493 | 1.00125.95 | |
| | 4 | O | LEU | 24 | 125.338 | 50.615 | 53.099 | 1.00126.05 | |
| | 5 | CB | LEU | 24 | 123.008 | 50.020 | 54.477 | 1.00127.81 | |
| | 6 | CG | LEU | 24 | 121.748 | 50.062 | 55.337 | 1.00127.97 | |
| | 7 | CD1 | LEU | 24 | 121.898 | 49.121 | 56.526 | 1.00126.52 | |
| 15 | 8 | CD2 | LEU | 24 | 121.487 | 51.490 | 55.822 | 1.00127.81 | |
| | 9 | 1H | LEU | 24 | 122.251 | 49.292 | 51.984 | 1.00 25.00 | |
| | 10 | 2H | LEU | 24 | 121.021 | 50.239 | 52.677 | 1.00 25.00 | |
| | 11 | 3H | LEU | 24 | 121.929 | 50.798 | 51.366 | 1.00 25.00 | |
| | 12 | N | TRP | 25 | 124.208 | 51.008 | 51.190 | 1.00128.26 | |
| 20 | 13 | CA | TRP | 25 | 125.348 | 50.953 | 50.308 | 1.00126.64 | |
| | 14 | C | TRP | 25 | 125.910 | 52.322 | 49.937 | 1.00128.50 | |
| | 15 | O | TRP | 25 | 127.131 | 52.480 | 49.824 | 1.00130.12 | |
| | 16 | CB | TRP | 25 | 124.945 | 50.134 | 49.078 | 1.00122.57 | |
| | 17 | CG | TRP | 25 | 124.537 | 48.725 | 49.460 | 1.00116.55 | |
| 25 | 18 | CD1 | TRP | 25 | 123.263 | 48.214 | 49.513 | 1.00111.25 | |
| | 19 | CD2 | TRP | 25 | 125.407 | 47.685 | 49.877 | 1.00114.36 | |
| | 20 | NE1 | TRP | 25 | 123.302 | 46.911 | 49.947 | 1.00109.76 | |
| | 21 | CE2 | TRP | 25 | 124.612 | 46.556 | 50.178 | 1.00113.64 | |
| | 22 | CE3 | TRP | 25 | 126.801 | 47.577 | 50.036 | 1.00114.01 | |
| 30 | 23 | CZ2 | TRP | 25 | 125.146 | 45.346 | 50.624 | 1.00114.93 | |
| | 24 | CZ3 | TRP | 25 | 127.340 | 46.387 | 50.476 | 1.00112.58 | |
| | 25 | CH2 | TRP | 25 | 126.515 | 45.282 | 50.767 | 1.00114.08 | |
| | 26 | H | TRP | 25 | 123.358 | 51.275 | 50.804 | 1.00 25.00 | |
| | 27 | HE1 | TRP | 25 | 122.575 | 46.258 | 50.073 | 1.00 25.00 | |
| 35 | 28 | N | GLY | 26 | 125.028 | 53.306 | 49.785 | 1.00129.69 | |
| | 29 | CA | GLY | 26 | 125.460 | 54.647 | 49.432 | 1.00129.22 | |
| | 30 | C | GLY | 26 | 126.079 | 54.744 | 48.049 | 1.00128.72 | |
| | 31 | O | GLY | 26 | 125.794 | 53.929 | 47.177 | 1.00128.98 | |
| | 32 | H | GLY | 26 | 124.083 | 53.132 | 49.888 | 1.00 25.00 | |
| 40 | 33 | N | ASP | 27 | 126.962 | 55.721 | 47.868 | 1.00128.05 | |
| | 34 | CA | ASP | 27 | 127.635 | 55.946 | 46.589 | 1.00126.16 | |
| | 35 | C | ASP | 27 | 128.786 | 54.971 | 46.340 | 1.00122.14 | |
| | 36 | O | ASP | 27 | 129.641 | 55.215 | 45.485 | 1.00121.90 | |
| | 37 | CB | ASP | 27 | 128.154 | 57.390 | 46.495 | 1.00128.56 | |
| 45 | 38 | CG | ASP | 27 | 127.036 | 58.414 | 46.382 | 1.00129.57 | |
| | 39 | OD1 | ASP | 27 | 126.092 | 58.200 | 45.590 | 1.00129.32 | |
| | 40 | OD2 | ASP | 27 | 127.109 | 59.446 | 47.083 | 1.00128.42 | |
| | 41 | H | ASP | 27 | 127.188 | 56.294 | 48.627 | 1.00 25.00 | |
| | 42 | N | GLN | 28 | 128.786 | 53.863 | 47.075 | 1.00117.67 | |
| 50 | 43 | CA | GLN | 28 | 129.811 | 52.833 | 46.950 | 1.00112.25 | |
| | 44 | C | GLN | 28 | 129.807 | 52.195 | 45.554 | 1.00112.76 | |

| | | | | | | | | |
|----|----|------|-----|-----|---------|--------|--------|------------|
| | 45 | O | GLN | 28 | 130.803 | 51.612 | 45.131 | 1.00110.25 |
| | 46 | CB | GLN | 28 | 129.581 | 51.764 | 48.025 | 1.00106.94 |
| | 47 | CG | GLN | 28 | 130.657 | 50.691 | 48.117 | 1.00101.12 |
| 5 | 48 | CD | GLN | 28 | 130.380 | 49.637 | 49.179 | 1.00 99.15 |
| | 49 | OE1 | GLN | 28 | 131.021 | 48.585 | 49.199 | 1.00 98.20 |
| | 50 | NE2 | GLN | 28 | 129.431 | 49.911 | 50.072 | 1.00 95.39 |
| | 51 | H | GLN | 28 | 128.073 | 53.736 | 47.724 | 1.00 25.00 |
| | 52 | 1HE2 | GLN | 28 | 129.287 | 49.206 | 50.749 | 1.00 25.00 |
| 10 | 53 | 2HE2 | GLN | 28 | 128.922 | 50.738 | 50.067 | 1.00 25.00 |
| | 54 | N | PHE | 29 | 128.696 | 52.349 | 44.833 | 1.00116.96 |
| | 55 | CA | PHE | 29 | 128.536 | 51.766 | 43.496 | 1.00118.70 |
| | 56 | C | PHE | 29 | 128.026 | 52.717 | 42.398 | 1.00122.05 |
| | 57 | O | PHE | 29 | 127.643 | 52.249 | 41.318 | 1.00123.10 |
| | 58 | CB | PHE | 29 | 127.570 | 50.572 | 43.539 | 1.00114.02 |
| 15 | 59 | CG | PHE | 29 | 127.906 | 49.532 | 44.568 | 1.00111.57 |
| | 60 | CD1 | PHE | 29 | 128.928 | 48.614 | 44.349 | 1.00109.61 |
| | 61 | CD2 | PHE | 29 | 127.148 | 49.429 | 45.731 | 1.00108.83 |
| | 62 | CE1 | PHE | 29 | 129.193 | 47.609 | 45.274 | 1.00102.49 |
| | 63 | CE2 | PHE | 29 | 127.401 | 48.432 | 46.663 | 1.00101.60 |
| 20 | 64 | CZ | PHE | 29 | 128.425 | 47.514 | 46.434 | 1.00101.60 |
| | 65 | H | PHE | 29 | 127.985 | 52.899 | 45.209 | 1.00 25.00 |
| | 66 | N | LEU | 30 | 127.984 | 54.022 | 42.669 | 1.00124.46 |
| | 67 | CA | LEU | 30 | 127.509 | 55.009 | 41.689 | 1.00127.15 |
| | 68 | C | LEU | 30 | 128.208 | 54.874 | 40.335 | 1.00128.12 |
| 25 | 69 | O | LEU | 30 | 127.578 | 54.916 | 39.277 | 1.00126.56 |
| | 70 | CB | LEU | 30 | 127.732 | 56.433 | 42.230 | 1.00128.23 |
| | 71 | CG | LEU | 30 | 127.357 | 57.672 | 41.388 | 1.00129.74 |
| | 72 | CD1 | LEU | 30 | 126.987 | 58.843 | 42.316 | 1.00126.98 |
| | 73 | CD2 | LEU | 30 | 128.437 | 58.089 | 40.428 | 1.00126.72 |
| 30 | 74 | H | LEU | 30 | 128.261 | 54.333 | 43.538 | 1.00 25.00 |
| | 75 | N | SER | 331 | 129.527 | 54.725 | 40.400 | 1.00129.78 |
| | 76 | CA | SER | 31 | 130.384 | 54.608 | 39.222 | 1.00130.48 |
| | 77 | C | SER | 31 | 131.618 | 53.722 | 39.458 | 1.00129.14 |
| | 78 | O | SER | 31 | 132.211 | 53.745 | 40.535 | 1.00127.41 |
| 35 | 79 | CB | SER | 31 | 130.831 | 56.004 | 38.781 | 1.00133.08 |
| | 80 | OG | SER | 31 | 131.461 | 56.700 | 39.845 | 1.00136.17 |
| | 81 | H | SER | 31 | 129.890 | 54.673 | 41.303 | 1.00 25.00 |
| | 82 | HG | SER | 31 | 130.880 | 56.771 | 40.611 | 1.00 25.00 |
| | 83 | N | PHE | 32 | 132.004 | 52.973 | 38.423 | 1.00127.29 |
| 40 | 84 | CA | PHE | 32 | 133.156 | 52.065 | 38.458 | 1.00126.38 |
| | 85 | C | PHE | 32 | 134.056 | 52.249 | 37.231 | 1.00129.92 |
| | 86 | O | PHE | 32 | 133.693 | 51.847 | 36.122 | 1.00131.71 |
| | 87 | CB | PHE | 32 | 132.683 | 50.601 | 38.531 | 1.00120.86 |
| | 88 | CG | PHE | 32 | 133.805 | 49.581 | 38.475 | 1.00117.02 |
| 45 | 89 | CD1 | PHE | 32 | 134.736 | 49.488 | 39.507 | 1.00114.77 |
| | 90 | CD2 | PHE | 32 | 133.912 | 48.701 | 37.396 | 1.00113.67 |
| | 91 | CE1 | PHE | 32 | 135.755 | 48.533 | 39.472 | 1.00111.21 |
| | 92 | CE2 | PHE | 32 | 134.927 | 47.742 | 37.349 | 1.00111.87 |
| | 93 | CZ | PHE | 32 | 135.851 | 47.658 | 38.389 | 1.00111.43 |
| 50 | 94 | H | PHE | 32 | 131.485 | 53.046 | 37.602 | 1.00 25.00 |
| | 95 | N | SER | 33 | 135.219 | 52.861 | 37.434 | 1.00129.98 |
| | 96 | CA | SER | 33 | 136.179 | 53.082 | 36.355 | 1.00128.55 |

| | | | | | | | | |
|----|-----|------|-----|----|---------|--------|--------|------------|
| | 97 | C | SER | 33 | 137.014 | 51.819 | 36.136 | 1.00128.72 |
| | 98 | O | SER | 33 | 137.973 | 51.561 | 36.865 | 1.00128.38 |
| | 99 | CB | SER | 33 | 137.079 | 54.277 | 36.684 | 1.00130.20 |
| 5 | 100 | OG | SER | 33 | 137.554 | 54.211 | 38.019 | 1.00130.89 |
| | 101 | H | SER | 33 | 135.440 | 53.163 | 38.329 | 1.00 25.00 |
| | 102 | HG | SER | 33 | 136.817 | 54.182 | 38.626 | 1.00 25.00 |
| | 103 | N | ILE | 34 | 136.616 | 51.017 | 35.153 | 1.00128.06 |
| | 104 | CA | ILE | 34 | 137.313 | 49.773 | 34.842 | 1.00127.26 |
| 10 | 105 | C | ILE | 34 | 138.715 | 50.001 | 34.268 | 1.00128.81 |
| | 106 | O | ILE | 34 | 138.869 | 50.556 | 33.177 | 1.00132.56 |
| | 107 | CB | ILE | 34 | 136.483 | 48.884 | 33.865 | 1.00125.22 |
| | 108 | CG1 | ILE | 34 | 137.227 | 47.570 | 33.595 | 1.00124.19 |
| | 109 | CG2 | ILE | 34 | 136.174 | 49.640 | 32.570 | 1.00123.27 |
| | 110 | CD1 | ILE | 34 | 136.518 | 46.611 | 32.665 | 1.00121.43 |
| 15 | 111 | H | ILE | 34 | 135.838 | 51.274 | 34.627 | 1.00 25.00 |
| | 112 | N | ASP | 35 | 139.736 | 49.600 | 35.020 | 1.00125.91 |
| | 113 | CA | ASP | 35 | 141.105 | 49.749 | 34.548 | 1.00120.92 |
| | 114 | C | ASP | 35 | 141.437 | 48.728 | 33.464 | 1.00116.38 |
| | 115 | O | ASP | 35 | 141.993 | 47.661 | 33.726 | 1.00115.56 |
| 20 | 116 | CB | ASP | 35 | 142.122 | 49.709 | 35.700 | 1.00122.56 |
| | 117 | CG | ASP | 35 | 141.780 | 48.684 | 36.761 | 1.00123.82 |
| | 118 | OD1 | ASP | 35 | 141.342 | 47.566 | 36.414 | 1.00129.46 |
| | 119 | OD2 | ASP | 35 | 141.952 | 49.002 | 37.955 | 1.00123.01 |
| | 120 | H | ASP | 35 | 139.577 | 49.234 | 35.909 | 1.00 25.00 |
| 25 | 121 | N | ASN | 36 | 141.017 | 49.067 | 32.254 | 1.00111.08 |
| | 122 | CA | ASN | 36 | 141.237 | 48.307 | 31.037 | 1.00107.72 |
| | 123 | C | ASN | 36 | 142.508 | 47.462 | 30.983 | 1.00104.04 |
| | 124 | O | ASN | 36 | 142.486 | 46.361 | 30.443 | 1.00103.31 |
| | 125 | CB | ASN | 36 | 141.160 | 49.215 | 29.783 | 1.00108.78 |
| 30 | 126 | CG | ASN | 36 | 141.378 | 50.742 | 30.076 | 1.00113.72 |
| | 127 | OD1 | ASN | 36 | 141.308 | 51.535 | 29.156 | 1.00115.16 |
| | 128 | ND2 | ASN | 36 | 141.666 | 51.127 | 31.309 | 1.00113.86 |
| | 129 | H | ASN | 36 | 140.490 | 49.899 | 32.196 | 1.00 25.00 |
| | 130 | 1HD2 | ASN | 36 | 141.642 | 52.070 | 31.558 | 1.00 25.00 |
| 35 | 131 | 2HD2 | ASN | 36 | 141.817 | 50.557 | 32.067 | 1.00 25.00 |
| | 132 | N | GLN | 37 | 143.593 | 47.958 | 31.571 | 1.00101.33 |
| | 133 | CA | GLN | 37 | 144.857 | 47.226 | 31.576 | 1.00 97.84 |
| | 134 | C | GLN | 37 | 144.752 | 45.887 | 32.306 | 1.00 91.48 |
| | 135 | O | GLN | 37 | 145.120 | 44.848 | 31.756 | 1.00 87.36 |
| 40 | 136 | CB | GLN | 37 | 145.964 | 48.079 | 32.204 | 1.00104.38 |
| | 137 | CG | GLN | 37 | 147.329 | 47.907 | 31.541 | 1.00109.27 |
| | 138 | CD | GLN | 37 | 147.433 | 48.643 | 30.213 | 1.00112.48 |
| | 139 | OE1 | GLN | 37 | 148.192 | 49.604 | 30.088 | 1.00116.42 |
| | 140 | NE2 | GLN | 37 | 146.670 | 48.202 | 29.220 | 1.00113.85 |
| 45 | 141 | H | GLN | 37 | 143.558 | 48.839 | 31.989 | 1.00 25.00 |
| | 142 | 1HE2 | GLN | 37 | 146.735 | 48.687 | 28.371 | 1.00 25.00 |
| | 143 | 2HE2 | GLN | 37 | 146.083 | 47.436 | 29.358 | 1.00 25.00 |
| | 144 | N | VAL | 38 | 144.242 | 45.916 | 33.536 | 1.00 85.52 |
| | 145 | CA | VAL | 38 | 144.092 | 44.702 | 34.337 | 1.00 79.25 |
| 50 | 146 | C | VAL | 38 | 143.148 | 43.731 | 33.634 | 1.00 77.63 |
| | 147 | O | VAL | 38 | 143.416 | 42.529 | 33.568 | 1.00 78.06 |
| | 148 | CB | VAL | 38 | 143.542 | 45.018 | 35.752 | 1.00 78.16 |

| | | | | | | | | | |
|----|-----|-----|-----|----|---------|--------|--------|------|--------|
| | 149 | CG1 | VAL | 38 | 143.484 | 43.754 | 36.593 | 1.00 | 75.39 |
| | 150 | CG2 | VAL | 38 | 144.409 | 46.061 | 36.437 | 1.00 | 78.10 |
| | 151 | H | VAL | 38 | 143.943 | 46.770 | 33.907 | 1.00 | 25.00 |
| | 152 | N | ALA | 39 | 142.060 | 44.268 | 33.086 | 1.00 | 71.24 |
| 5 | 153 | CA | ALA | 39 | 141.071 | 43.463 | 32.379 | 1.00 | 66.46 |
| | 154 | C | ALA | 39 | 141.694 | 42.736 | 31.191 | 1.00 | 65.26 |
| | 155 | O | ALA | 39 | 141.519 | 41.527 | 31.038 | 1.00 | 59.37 |
| | 156 | CB | ALA | 39 | 139.910 | 44.338 | 31.916 | 1.00 | 64.84 |
| | 157 | H | ALA | 39 | 141.924 | 45.233 | 33.161 | 1.00 | 25.00 |
| 10 | 158 | N | GLU | 40 | 142.436 | 43.472 | 30.366 | 1.00 | 66.68 |
| | 159 | CA | GLU | 40 | 143.086 | 42.896 | 29.190 | 1.00 | 69.85 |
| | 160 | C | GLU | 40 | 144.107 | 41.828 | 29.559 | 1.00 | 66.85 |
| | 161 | O | GLU | 40 | 144.233 | 40.818 | 28.859 | 1.00 | 65.59 |
| | 162 | CB | GLU | 40 | 143.744 | 43.985 | 28.342 | 1.00 | 75.56 |
| 15 | 163 | CG | GLU | 40 | 142.752 | 44.836 | 27.560 | 1.00 | 89.79 |
| | 164 | CD | GLU | 40 | 143.409 | 45.993 | 26.828 | 1.00 | 98.34 |
| | 165 | OE1 | GLU | 40 | 144.515 | 45.807 | 26.273 | 1.00 | 101.87 |
| | 166 | OE2 | GLU | 40 | 142.814 | 47.092 | 26.808 | 1.00 | 102.72 |
| | 167 | H | GLU | 40 | 142.551 | 44.427 | 30.550 | 1.00 | 25.00 |
| 20 | 168 | N | LYS | 41 | 144.830 | 42.048 | 30.656 | 1.00 | 62.69 |
| | 169 | CA | LYS | 41 | 145.821 | 41.079 | 31.112 | 1.00 | 60.33 |
| | 170 | C | LYS | 41 | 145.081 | 39.798 | 31.478 | 1.00 | 56.90 |
| | 171 | O | LYS | 41 | 145.440 | 38.707 | 31.024 | 1.00 | 56.12 |
| | 172 | CB | LYS | 41 | 146.588 | 41.603 | 32.331 | 1.00 | 64.30 |
| 25 | 173 | CG | LYS | 41 | 147.689 | 40.655 | 32.802 | 1.00 | 70.61 |
| | 174 | CD | LYS | 41 | 148.373 | 41.137 | 34.070 | 1.00 | 74.86 |
| | 175 | CE | LYS | 41 | 149.449 | 40.152 | 34.505 | 1.00 | 79.07 |
| | 176 | NZ | LYS | 41 | 150.138 | 40.584 | 35.753 | 1.00 | 86.06 |
| | 177 | H | LYS | 41 | 144.700 | 42.879 | 31.160 | 1.00 | 25.00 |
| 30 | 178 | 1HZ | LYS | 41 | 150.588 | 41.510 | 35.601 | 1.00 | 25.00 |
| | 179 | 2HZ | LYS | 41 | 149.443 | 40.661 | 36.524 | 1.00 | 25.00 |
| | 180 | 3HZ | LYS | 41 | 150.864 | 39.885 | 36.010 | 1.00 | 25.00 |
| | 181 | N | TYR | 42 | 144.027 | 39.951 | 32.278 | 1.00 | 54.48 |
| | 182 | CA | TYR | 42 | 143.200 | 38.831 | 32.712 | 1.00 | 49.46 |
| 35 | 183 | C | TYR | 42 | 142.687 | 38.048 | 31.508 | 1.00 | 49.51 |
| | 184 | O | TYR | 42 | 142.886 | 36.837 | 31.418 | 1.00 | 46.83 |
| | 185 | CB | TYR | 42 | 142.011 | 39.332 | 33.535 | 1.00 | 49.09 |
| | 186 | CG | TYR | 42 | 142.316 | 39.665 | 34.981 | 1.00 | 51.81 |
| | 187 | CD1 | TYR | 42 | 143.609 | 39.555 | 35.498 | 1.00 | 55.25 |
| 40 | 188 | CD2 | TYR | 42 | 141.297 | 40.067 | 35.844 | 1.00 | 51.34 |
| | 189 | CE1 | TYR | 42 | 143.873 | 39.836 | 36.843 | 1.00 | 60.63 |
| | 190 | CE2 | TYR | 42 | 141.548 | 40.347 | 37.180 | 1.00 | 51.18 |
| | 191 | CZ | TYR | 42 | 142.832 | 40.231 | 37.677 | 1.00 | 57.44 |
| | 192 | OH | TYR | 42 | 143.064 | 40.503 | 39.009 | 1.00 | 57.29 |
| 45 | 193 | H | TYR | 42 | 143.796 | 40.855 | 32.582 | 1.00 | 25.00 |
| | 194 | HH | TYR | 42 | 142.245 | 40.765 | 39.435 | 1.00 | 25.00 |
| | 195 | N | ALA | 43 | 142.067 | 38.756 | 30.568 | 1.00 | 48.90 |
| | 196 | CA | ALA | 43 | 141.514 | 38.150 | 29.359 | 1.00 | 49.75 |
| | 197 | C | ALA | 43 | 142.560 | 37.363 | 28.576 | 1.00 | 49.98 |
| 50 | 198 | O | ALA | 43 | 142.331 | 36.209 | 28.204 | 1.00 | 49.38 |
| | 199 | CB | ALA | 43 | 140.897 | 39.223 | 28.477 | 1.00 | 46.66 |
| | 200 | H | ALA | 43 | 141.980 | 39.722 | 30.693 | 1.00 | 25.00 |

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|----|-----|------|-----|----|---------|--------|--------|------|-------|
| | 201 | N | GLN | 44 | 143.711 | 37.987 | 22.344 | 1.00 | 52.04 |
| | 202 | CA | GLN | 44 | 144.796 | 37.352 | 27.607 | 1.00 | 51.53 |
| | 203 | C | GLN | 44 | 145.219 | 36.030 | 28.257 | 1.00 | 45.51 |
| | 204 | O | GLN | 44 | 145.304 | 35.002 | 27.582 | 1.00 | 43.18 |
| 5 | 205 | CB | GLN | 44 | 145.994 | 38.299 | 27.506 | 1.00 | 58.59 |
| | 206 | CG | GLN | 44 | 147.101 | 37.804 | 26.583 | 1.00 | 74.05 |
| | 207 | CD | GLN | 44 | 148.364 | 38.649 | 26.658 | 1.00 | 84.03 |
| | 208 | OE1 | GLN | 44 | 148.343 | 39.784 | 27.132 | 1.00 | 90.02 |
| | 209 | NE2 | GLN | 44 | 149.475 | 38.092 | 26.187 | 1.00 | 84.98 |
| 10 | 210 | H | GLN | 44 | 143.837 | 38.900 | 28.677 | 1.00 | 25.00 |
| | 211 | 1HE2 | GLN | 44 | 150.290 | 38.631 | 26.238 | 1.00 | 25.00 |
| | 212 | 2HE2 | GLN | 44 | 149.438 | 37.187 | 25.820 | 1.00 | 25.00 |
| | 213 | N | GLU | 45 | 145.466 | 36.047 | 29.565 | 1.00 | 40.03 |
| | 214 | CA | GLU | 45 | 145.874 | 34.831 | 30.261 | 1.00 | 37.78 |
| 15 | 215 | C | GLU | 45 | 144.740 | 33.813 | 30.320 | 1.00 | 41.99 |
| | 216 | O | GLU | 45 | 144.970 | 32.609 | 30.153 | 1.00 | 43.40 |
| | 217 | CB | GLU | 45 | 146.374 | 35.134 | 31.673 | 1.00 | 38.09 |
| | 218 | CG | GLU | 45 | 147.037 | 33.924 | 32.334 | 1.00 | 41.87 |
| | 219 | CD | GLU | 45 | 147.595 | 34.209 | 33.718 | 1.00 | 52.34 |
| 20 | 220 | OE1 | GLU | 45 | 147.678 | 35.393 | 34.116 | 1.00 | 58.77 |
| | 221 | OE2 | GLU | 45 | 147.962 | 33.235 | 34.409 | 1.00 | 53.14 |
| | 222 | H | GLU | 45 | 145.372 | 36.890 | 30.064 | 1.00 | 25.00 |
| | 223 | N | ILE | 46 | 143.521 | 34.296 | 30.553 | 1.00 | 38.09 |
| | 224 | CA | ILE | 46 | 142.352 | 33.428 | 30.622 | 1.00 | 35.19 |
| 25 | 225 | C | ILE | 46 | 142.239 | 32.630 | 29.328 | 1.00 | 37.05 |
| | 226 | O | ILE | 46 | 141.923 | 31.441 | 29.360 | 1.00 | 40.60 |
| | 227 | CB | ILE | 46 | 141.054 | 34.236 | 30.886 | 1.00 | 33.29 |
| | 228 | CG1 | ILE | 46 | 140.992 | 34.650 | 32.357 | 1.00 | 25.99 |
| | 229 | CG2 | ILE | 46 | 139.817 | 33.420 | 30.528 | 1.00 | 33.03 |
| 30 | 230 | CD1 | ILE | 46 | 139.889 | 35.630 | 32.667 | 1.00 | 27.20 |
| | 231 | H | ILE | 46 | 143.414 | 35.255 | 30.675 | 1.00 | 25.00 |
| | 232 | N | GLU | 47 | 142.548 | 33.263 | 28.199 | 1.00 | 37.32 |
| | 233 | CA | GLU | 47 | 142.485 | 32.581 | 26.910 | 1.00 | 43.67 |
| | 234 | C | GLU | 47 | 143.420 | 31.379 | 26.870 | 1.00 | 44.27 |
| 35 | 235 | O | GLU | 47 | 143.061 | 30.324 | 26.341 | 1.00 | 48.49 |
| | 236 | CB | GLU | 47 | 142.817 | 33.537 | 25.765 | 1.00 | 50.83 |
| | 237 | CG | GLU | 47 | 141.700 | 34.516 | 25.422 | 1.00 | 72.13 |
| | 238 | CD | GLU | 47 | 140.408 | 33.833 | 24.970 | 1.00 | 80.45 |
| | 239 | OE1 | GLU | 47 | 140.440 | 32.643 | 24.577 | 1.00 | 82.39 |
| 40 | 240 | OE2 | GLU | 47 | 139.353 | 34.501 | 25.001 | 1.00 | 87.14 |
| | 241 | H | GLU | 47 | 142.813 | 34.208 | 28.233 | 1.00 | 25.00 |
| | 242 | N | ALA | 48 | 144.610 | 31.538 | 27.444 | 1.00 | 41.56 |
| | 243 | CA | ALA | 48 | 145.597 | 30.464 | 27.489 | 1.00 | 36.13 |
| | 244 | C | ALA | 48 | 145.078 | 29.340 | 28.375 | 1.00 | 38.33 |
| 45 | 245 | O | ALA | 48 | 145.027 | 28.176 | 27.964 | 1.00 | 40.71 |
| | 246 | CB | ALA | 48 | 146.917 | 30.990 | 28.031 | 1.00 | 33.18 |
| | 247 | H | ALA | 48 | 144.824 | 32.404 | 27.853 | 1.00 | 25.00 |
| | 248 | N | LEU | 49 | 144.662 | 29.708 | 29.583 | 1.00 | 37.02 |
| | 249 | CA | LEU | 49 | 144.136 | 28.757 | 30.554 | 1.00 | 34.21 |
| 50 | 250 | C | LEU | 49 | 142.894 | 28.044 | 30.029 | 1.00 | 33.34 |
| | 251 | O | LEU | 49 | 142.694 | 26.860 | 30.296 | 1.00 | 34.71 |
| | 252 | CB | LEU | 49 | 143.816 | 29.477 | 31.862 | 1.00 | 32.92 |

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|----|-----|------|-----|----|---------|--------|---------|------|-------|
| | 253 | CG | LEU | 49 | 145.013 | 30.132 | 32.551 | 1.00 | 29.78 |
| | 254 | CD1 | LEU | 49 | 144.541 | 31.096 | 33.621 | 1.00 | 28.55 |
| | 255 | CD2 | LEU | 49 | 145.915 | 29.062 | 33.139 | 1.00 | 31.11 |
| | 256 | H | LEU | 49 | 144.717 | 30.657 | 29.827 | 1.00 | 25.00 |
| 5 | 257 | N | LYS | 50 | 142.083 | 28.759 | 29.254 | 1.00 | 35.43 |
| | 258 | CA | LYS | 50 | 140.858 | 28.208 | 28.681 | 1.00 | 36.99 |
| | 259 | C | LYS | 50 | 141.193 | 27.105 | 27.687 | 1.00 | 39.13 |
| | 260 | O | LYS | 50 | 140.643 | 26.004 | 27.762 | 1.00 | 39.46 |
| | 261 | CB | LYS | 50 | 140.056 | 29.307 | 27.981 | 1.00 | 38.20 |
| 10 | 262 | CG | LYS | 50 | 138.670 | 28.882 | 27.520 | 1.00 | 37.82 |
| | 263 | CD | LYS | 50 | 138.021 | 29.947 | 26.638 | 1.00 | 41.56 |
| | 264 | CE | LYS | 50 | 137.926 | 31.297 | 27.341 | 1.00 | 44.73 |
| | 265 | NZ | LYS | 50 | 137.282 | 32.342 | 26.489 | 1.00 | 40.08 |
| | 266 | H | LYS | 50 | 142.323 | 29.682 | 29.055 | 1.00 | 25.00 |
| 15 | 267 | 1HZ | LYS | 50 | 136.318 | 32.042 | 26.239 | 1.00 | 25.00 |
| | 268 | 2HZ | LYS | 50 | 137.245 | 33.240 | 27.012 | 1.00 | 25.00 |
| | 269 | 3HZ | LYS | 50 | 137.841 | 32.474 | 25.620 | 1.00 | 25.00 |
| | 270 | N | GLU | 51 | 142.106 | 27.396 | 26.765 | 1.00 | 41.23 |
| | 271 | CA | GLU | 51 | 142.516 | 26.419 | 25.762 | 1.00 | 44.62 |
| 20 | 272 | C | GLU | 51 | 143.174 | 25.226 | 26.446 | 1.00 | 42.95 |
| | 273 | O | GLU | 51 | 142.931 | 24.073 | 26.091 | 1.00 | 43.13 |
| | 274 | CB | GLU | 51 | 143.489 | 27.055 | 24.766 | 1.00 | 52.90 |
| | 275 | CG | GLU | 51 | 143.846 | 26.162 | 23.581 | 1.00 | 70.21 |
| | 276 | CD | GLU | 51 | 142.623 | 25.709 | 22.792 | 1.00 | 79.98 |
| 25 | 277 | OE1 | GLU | 51 | 141.917 | 26.575 | 22.226 | 1.00 | 86.16 |
| | 278 | OE2 | GLU | 51 | 142.368 | 24.486 | 22.739 | 1.00 | 81.08 |
| | 279 | H | GLU | 51 | 142.510 | 28.293 | 26.751 | 1.00 | 25.00 |
| | 280 | N | GLN | 52 | 143.965 | 25.514 | 27.471 | 1.00 | 48.21 |
| | 281 | CA | GLN | 52 | 144.662 | 24.480 | 28.223 | 1.00 | 49.28 |
| 30 | 282 | C | GLN | 52 | 143.657 | 23.563 | 28.933 | 1.00 | 44.99 |
| | 283 | O | GLN | 52 | 143.817 | 22.337 | 28.936 | 1.00 | 42.93 |
| | 284 | CB | GLN | 52 | 145.609 | 25.138 | 29.230 | 1.00 | 51.94 |
| | 285 | CG | GLN | 52 | 146.728 | 24.247 | 29.736 | 1.00 | 57.86 |
| | 286 | CD | GLN | 52 | 147.655 | 24.973 | 30.696 | 1.00 | 61.66 |
| 35 | 287 | OE1 | GLN | 52 | 147.719 | 26.205 | 30.711 | 1.00 | 53.55 |
| | 288 | NE2 | GLN | 52 | 148.372 | 24.211 | 31.511 | 1.00 | 66.48 |
| | 289 | H | GLN | 52 | 144.095 | 26.453 | 27.720 | 1.00 | 25.00 |
| | 290 | 1HE2 | GLN | 52 | 148.989 | 24.676 | 32.114 | 1.00 | 25.00 |
| | 291 | 2HE2 | GLN | 52 | 148.283 | 23.237 | 31.480 | 1.00 | 25.00 |
| 40 | 292 | N | THR | 53 | 142.615 | 24.160 | 29.512 | 1.00 | 42.37 |
| | 293 | CA | THR | 53 | 141.578 | 23.404 | 30.214 | 1.00 | 41.44 |
| | 294 | C | THR | 53 | 140.753 | 22.584 | 29.220 | 1.00 | 40.96 |
| | 295 | O | THR | 53 | 140.334 | 21.462 | 29.519 | 1.00 | 38.12 |
| | 296 | CB | THR | 53 | 140.648 | 24.338 | 31.027 | 1.00 | 42.33 |
| 45 | 297 | OG1 | THR | 53 | 141.420 | 25.054 | 32.001 | 1.00 | 42.93 |
| | 298 | CG2 | THR | 53 | 139.569 | 23.534 | 31.746 | 1.00 | 41.61 |
| | 299 | H | THR | 53 | 142.537 | 25.134 | 29.467 | 1.00 | 25.00 |
| | 300 | HG1 | THR | 53 | 142.088 | 25.586 | 31.555 | 1.00 | 25.00 |
| | 301 | N | ARG | 54 | 140.553 | 23.138 | 28.027 | 1.00 | 42.45 |
| 50 | 302 | CA | ARG | 54 | 139.802 | 22.461 | 26.9976 | 1.00 | 41.46 |
| | 303 | C | ARG | 54 | 140.516 | 21.152 | 26.653 | 1.00 | 43.94 |
| | 304 | O | ARG | 54 | 139.891 | 20.088 | 26.607 | 1.00 | 41.93 |

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|----|-----|------|-----|----|---------|--------|--------|------|-------|
| | 305 | CB | ARG | 54 | 139.731 | 23.344 | 25.727 | 1.00 | 43.17 |
| | 306 | CG | ARG | 54 | 138.759 | 22.861 | 24.658 | 1.00 | 49.52 |
| | 307 | CD | ARG | 54 | 138.792 | 23.763 | 23.428 | 1.00 | 55.06 |
| | 308 | NE | ARG | 54 | 138.600 | 25.176 | 23.764 | 1.00 | 65.13 |
| 5 | 309 | CZ | ARG | 54 | 137.416 | 25.758 | 23.951 | 1.00 | 73.50 |
| | 310 | NH1 | ARG | 54 | 136.293 | 25.058 | 23.836 | 1.00 | 78.69 |
| | 311 | NH2 | ARG | 54 | 137.353 | 27.046 | 24.263 | 1.00 | 72.72 |
| | 312 | H | ARG | 54 | 140.919 | 24.030 | 27.846 | 1.00 | 25.00 |
| | 313 | HE | ARG | 54 | 139.400 | 25.734 | 23.857 | 1.00 | 25.00 |
| 10 | 314 | 1HH1 | ARG | 54 | 136.328 | 24.086 | 23.604 | 1.00 | 25.00 |
| | 315 | 2HH1 | ARG | 54 | 135.410 | 25.505 | 23.976 | 1.00 | 25.00 |
| | 316 | 1HH2 | ARG | 54 | 138.196 | 27.578 | 24.357 | 1.00 | 25.00 |
| | 317 | 2HH2 | ARG | 54 | 136.466 | 27.484 | 24.403 | 1.00 | 25.00 |
| | 318 | N | SER | 55 | 141.834 | 21.233 | 26.480 | 1.00 | 41.53 |
| 15 | 319 | CA | SER | 55 | 142.645 | 20.062 | 26.176 | 1.00 | 41.04 |
| | 320 | C | SER | 55 | 142.550 | 19.010 | 27.284 | 1.00 | 42.34 |
| | 321 | O | SER | 55 | 142.587 | 17.810 | 27.005 | 1.00 | 42.66 |
| | 322 | CB | SER | 55 | 144.100 | 20.469 | 25.916 | 1.00 | 46.50 |
| | 323 | OG | SER | 55 | 144.208 | 21.230 | 24.719 | 1.00 | 41.12 |
| 20 | 324 | H | SER | 55 | 142.280 | 22.107 | 26.538 | 1.00 | 25.00 |
| | 325 | HG | SER | 55 | 143.898 | 20.704 | 23.977 | 1.00 | 25.00 |
| | 326 | N | MET | 56 | 142.399 | 19.458 | 28.531 | 1.00 | 41.33 |
| | 327 | CA | MET | 56 | 142.265 | 18.544 | 29.668 | 1.00 | 40.87 |
| | 328 | C | MET | 56 | 141.003 | 17.703 | 29.501 | 1.00 | 43.46 |
| 25 | 329 | O | MET | 56 | 141.017 | 16.489 | 29.711 | 1.00 | 41.72 |
| | 330 | CB | MET | 56 | 142.164 | 19.312 | 30.989 | 1.00 | 44.45 |
| | 331 | CG | MET | 56 | 143.461 | 19.894 | 31.500 | 1.00 | 46.36 |
| | 332 | SD | MET | 56 | 143.231 | 20.659 | 33.118 | 1.00 | 45.60 |
| | 333 | CE | MET | 56 | 143.715 | 22.320 | 32.763 | 1.00 | 44.30 |
| 30 | 334 | H | MET | 56 | 142.383 | 20.426 | 28.690 | 1.00 | 25.00 |
| | 335 | N | LEU | 57 | 139.910 | 18.365 | 29.132 | 1.00 | 42.82 |
| | 336 | CA | LEU | 57 | 138.632 | 17.696 | 28.929 | 1.00 | 41.38 |
| | 337 | C | LEU | 57 | 138.684 | 16.700 | 27.779 | 1.00 | 43.36 |
| | 338 | O | LEU | 57 | 138.042 | 15.653 | 27.831 | 1.00 | 45.75 |
| 35 | 339 | CB | LEU | 57 | 137.531 | 18.726 | 28.670 | 1.00 | 34.91 |
| | 340 | CG | LEU | 57 | 137.047 | 19.512 | 29.887 | 1.00 | 31.36 |
| | 341 | CD1 | LEU | 57 | 136.174 | 20.663 | 29.441 | 1.00 | 31.29 |
| | 342 | CD2 | LEU | 57 | 136.287 | 18.592 | 30.833 | 1.00 | 25.33 |
| | 343 | H | LEU | 57 | 139.968 | 19.335 | 28.990 | 1.00 | 25.00 |
| 40 | 344 | N | LEU | 58 | 139.466 | 17.016 | 26.754 | 1.00 | 43.66 |
| | 345 | CA | LEU | 58 | 139.577 | 16.145 | 25.591 | 1.00 | 48.27 |
| | 346 | C | LEU | 58 | 140.659 | 15.059 | 25.683 | 1.00 | 53.11 |
| | 347 | O | LEU | 58 | 141.005 | 14.441 | 24.672 | 1.00 | 54.87 |
| | 348 | CB | LEU | 58 | 139.762 | 16.987 | 24.325 | 1.00 | 45.38 |
| 45 | 349 | CG | LEU | 58 | 138.682 | 18.051 | 24.083 | 1.00 | 48.84 |
| | 350 | CD1 | LEU | 58 | 138.936 | 18.772 | 22.772 | 1.00 | 46.56 |
| | 351 | CD2 | LEU | 58 | 137.303 | 17.413 | 24.074 | 1.00 | 49.64 |
| | 352 | H | LEU | 58 | 139.978 | 17.851 | 26.781 | 1.00 | 25.00 |
| | 353 | N | ALA | 59 | 141.180 | 14.813 | 26.884 | 1.00 | 58.17 |
| 50 | 354 | CA | ALA | 59 | 142.208 | 13.788 | 27.078 | 1.00 | 61.28 |
| | 355 | C | ALA | 59 | 141.605 | 12.397 | 26.874 | 1.00 | 66.17 |
| | 356 | O | ALA | 59 | 140.672 | 11.998 | 27.572 | 1.00 | 65.17 |

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|----|-----|------|-----|----|---------|--------|--------|------|-------|
| | 357 | CB | ALA | 59 | 142.830 | 13.908 | 28.460 | 1.00 | 61.08 |
| | 358 | H | ALA | 59 | 140.859 | 15.316 | 27.661 | 1.00 | 25.00 |
| | 359 | N | THR | 60 | 142.188 | 11.651 | 25.943 | 1.00 | 71.93 |
| | 360 | CA | THR | 60 | 141.717 | 10.317 | 25.572 | 1.00 | 78.50 |
| 5 | 361 | C | THR | 60 | 141.721 | 9.179 | 26.599 | 1.00 | 77.85 |
| | 362 | O | THR | 60 | 140.694 | 8.536 | 26.812 | 1.00 | 82.48 |
| | 363 | CB | THR | 60 | 142.443 | 9.828 | 24.304 | 1.00 | 80.20 |
| | 364 | OG1 | THR | 60 | 143.852 | 10.053 | 24.449 | 1.00 | 82.38 |
| | 365 | CG2 | THR | 60 | 141.933 | 10.573 | 23.076 | 1.00 | 82.60 |
| 10 | 366 | H | THR | 60 | 142.957 | 12.026 | 25.478 | 1.00 | 25.00 |
| | 367 | HG1 | THR | 60 | 144.029 | 10.991 | 24.540 | 1.00 | 25.00 |
| | 368 | N | GLY | 61 | 142.866 | 8.914 | 27.217 | 1.00 | 74.94 |
| | 369 | CA | GLY | 61 | 142.942 | 7.813 | 28.165 | 1.00 | 75.87 |
| | 370 | C | GLY | 61 | 142.662 | 8.104 | 29.626 | 1.00 | 73.64 |
| 15 | 371 | O | GLY | 61 | 143.494 | 7.804 | 30.484 | 1.00 | 73.89 |
| | 372 | H | GLY | 61 | 143.654 | 9.465 | 27.047 | 1.00 | 25.00 |
| | 373 | N | ARG | 62 | 141.491 | 8.651 | 29.925 | 1.00 | 70.85 |
| | 374 | CA | ARG | 62 | 141.149 | 8.960 | 31.307 | 1.00 | 67.41 |
| | 375 | C | ARG | 62 | 140.068 | 8.054 | 31.870 | 1.00 | 61.77 |
| 20 | 376 | O | ARG | 62 | 139.147 | 7.654 | 31.160 | 1.00 | 63.43 |
| | 377 | CB | ARG | 62 | 140.755 | 10.429 | 31.444 | 1.00 | 69.30 |
| | 378 | CG | ARG | 62 | 141.883 | 11.309 | 31.967 | 1.00 | 75.81 |
| | 379 | CD | ARG | 62 | 141.666 | 12.780 | 31.647 | 1.00 | 78.22 |
| | 380 | NE | ARG | 62 | 140.334 | 13.254 | 32.009 | 1.00 | 79.69 |
| 25 | 381 | CZ | ARG | 62 | 139.335 | 13.405 | 31.143 | 1.00 | 88.12 |
| | 382 | NH1 | ARG | 62 | 139.508 | 13.118 | 29.859 | 1.00 | 90.62 |
| | 383 | NH2 | ARG | 62 | 138.160 | 13.852 | 31.559 | 1.00 | 92.99 |
| | 384 | H | ARG | 62 | 140.835 | 8.835 | 29.218 | 1.00 | 25.00 |
| | 385 | HE | ARG | 62 | 140.163 | 13.477 | 32.948 | 1.00 | 25.00 |
| 30 | 386 | 1HH1 | ARG | 62 | 140.393 | 12.785 | 29.534 | 1.00 | 25.00 |
| | 387 | 2HH1 | ARG | 62 | 138.752 | 13.233 | 29.216 | 1.00 | 25.00 |
| | 388 | 1HH2 | ARG | 62 | 138.022 | 14.076 | 32.524 | 1.00 | 25.00 |
| | 389 | 2HH2 | ARG | 62 | 137.408 | 13.963 | 30.909 | 1.00 | 25.00 |
| | 390 | N | LYS | 63 | 140.214 | 7.702 | 33.143 | 1.00 | 56.71 |
| 35 | 391 | CA | LYS | 63 | 139.258 | 6.840 | 33.830 | 1.00 | 53.88 |
| | 392 | C | LYS | 63 | 137.986 | 7.614 | 34.170 | 1.00 | 49.91 |
| | 393 | O | LYS | 63 | 138.024 | 8.831 | 34.377 | 1.00 | 43.13 |
| | 394 | CB | LYS | 63 | 139.876 | 6.284 | 35.114 | 1.00 | 60.17 |
| | 395 | CG | LYS | 63 | 141.181 | 5.544 | 34.901 | 1.00 | 72.02 |
| 40 | 396 | CD | LYS | 63 | 141.807 | 5.141 | 36.225 | 1.00 | 82.26 |
| | 397 | CE | LYS | 63 | 143.131 | 4.428 | 36.004 | 1.00 | 90.54 |
| | 398 | NZ | LYS | 63 | 143.764 | 4.015 | 37.286 | 1.00 | 94.67 |
| | 399 | H | LYS | 63 | 140.988 | 8.042 | 33.633 | 1.00 | 25.00 |
| | 400 | 1HZ | LYS | 63 | 143.130 | 3.366 | 37.795 | 1.00 | 25.00 |
| 45 | 401 | 2HZ | LYS | 63 | 144.664 | 3.533 | 37.085 | 1.00 | 25.00 |
| | 402 | 3HZ | LYS | 63 | 143.945 | 4.857 | 37.868 | 1.00 | 25.00 |
| | 403 | N | LEU | 64 | 136.877 | 6.890 | 34.289 | 1.00 | 44.28 |
| | 404 | CA | LEU | 64 | 135.583 | 7.487 | 34.603 | 1.00 | 40.75 |
| | 405 | C | LEU | 64 | 135.650 | 8.425 | 35.805 | 1.00 | 38.00 |
| 50 | 406 | O | LEU | 64 | 135.273 | 9.592 | 35.708 | 1.00 | 38.34 |
| | 407 | CB | LEU | 64 | 134.539 | 6.395 | 34.858 | 1.00 | 37.20 |
| | 408 | CG | LEU | 64 | 133.128 | 6.897 | 35.170 | 1.00 | 35.50 |

| | | | | | | | | | |
|----|-----|------|-----|----|---------|---------|--------|------|-------|
| | 409 | CD1 | LEU | 64 | 132.563 | 7.618 | 33.964 | 1.00 | 30.93 |
| | 410 | CD2 | LEU | 64 | 132.232 | 5.741 | 35.572 | 1.00 | 32.83 |
| | 411 | H | LEU | 64 | 136.930 | 5.926 | 34.145 | 1.00 | 25.00 |
| | 412 | N | ALA | 65 | 136.149 | 7.915 | 36.927 | 1.00 | 34.87 |
| 5 | 413 | CA | ALA | 65 | 136.264 | 8.700 | 38.152 | 1.00 | 33.63 |
| | 414 | C | ALA | 65 | 136.977 | 10.022 | 37.909 | 1.00 | 32.94 |
| | 415 | O | ALA | 65 | 136.508 | 11.073 | 38.342 | 1.00 | 31.36 |
| | 416 | CB | ALA | 65 | 136.991 | 7.900 | 39.222 | 1.00 | 26.54 |
| | 417 | H | ALA | 65 | 136.437 | 6.983 | 36.932 | 1.00 | 25.00 |
| 10 | 418 | N | ASP | 66 | 138.094 | 9.965 | 37.188 | 1.00 | 35.39 |
| | 419 | CA | ASP | 66 | 138.887 | 11.151 | 36.882 | 1.00 | 34.98 |
| | 420 | C | ASP | 66 | 138.127 | 12.136 | 36.002 | 1.00 | 34.90 |
| | 421 | O | ASP | 66 | 138.200 | 13.352 | 36.210 | 1.00 | 34.81 |
| | 422 | CB | ASP | 66 | 140.202 | 10.755 | 36.202 | 1.00 | 42.66 |
| 15 | 423 | CG | ASP | 66 | 141.054 | 9.825 | 37.059 | 1.00 | 51.98 |
| | 424 | OD1 | ASP | 66 | 141.008 | 9.934 | 38.306 | 1.00 | 48.05 |
| | 425 | OD2 | ASP | 66 | 141.774 | 8.982 | 36.479 | 1.00 | 59.40 |
| | 426 | H | ASP | 66 | 138.390 | 9.103 | 36.840 | 1.00 | 25.00 |
| | 427 | N | THR | 67 | 137.400 | 11.607 | 35.023 | 1.00 | 32.76 |
| 20 | 428 | CA | THR | 67 | 136.617 | 12.433 | 34.110 | 1.00 | 29.98 |
| | 429 | C | THR | 67 | 135.486 | 13.131 | 34.869 | 1.00 | 27.93 |
| | 430 | O | THR | 67 | 135.262 | 14.337 | 34.708 | 1.00 | 26.55 |
| | 431 | CB | THR | 67 | 136.033 | 11.582 | 32.963 | 1.00 | 33.36 |
| | 432 | OG1 | THR | 67 | 137.102 | 10.914 | 32.278 | 1.00 | 32.56 |
| 25 | 433 | CG2 | THR | 67 | 135.272 | 12.460 | 31.972 | 1.00 | 24.21 |
| | 434 | H | THR | 67 | 137.385 | 10.635 | 34.900 | 1.00 | 25.00 |
| | 435 | HG1 | THR | 67 | 136.746 | 10.375 | 31.566 | 1.00 | 25.00 |
| | 436 | N | LEU | 68 | 134.806 | 12.382 | 35.730 | 1.00 | 24.35 |
| | 437 | CA | LEU | 68 | 133.717 | 12.938 | 36.513 | 1.00 | 23.41 |
| 30 | 438 | C | LEU | 68 | 134.223 | 14.025 | 37.449 | 1.00 | 28.28 |
| | 439 | O | LEU | 68 | 133.644 | 15.112 | 37.507 | 1.00 | 26.82 |
| | 440 | CB | LEU | 68 | 133.004 | 11.842 | 37.301 | 1.00 | 24.43 |
| | 441 | CG | LEU | 68 | 132.221 | 10.8411 | 36.447 | 1.00 | 32.03 |
| | 442 | CD1 | LEU | 68 | 131.651 | 9.744 | 37.330 | 1.00 | 23.28 |
| 35 | 443 | CD2 | LEU | 68 | 131.112 | 11.556 | 35.680 | 1.00 | 27.61 |
| | 444 | H | LEU | 68 | 135.049 | 11.442 | 35.844 | 1.00 | 25.00 |
| | 445 | N | ASN | 69 | 135.323 | 13.750 | 38.147 | 1.00 | 26.79 |
| | 446 | CA | ASN | 69 | 135.894 | 14.724 | 39.072 | 1.00 | 30.78 |
| | 447 | C | ASN | 69 | 136.341 | 15.981 | 38.340 | 1.00 | 28.43 |
| 40 | 448 | O | ASN | 69 | 136.165 | 17.092 | 38.837 | 1.00 | 30.31 |
| | 449 | CB | ASN | 69 | 137.061 | 14.125 | 39.867 | 1.00 | 40.14 |
| | 450 | CG | ASN | 69 | 136.597 | 13.165 | 40.959 | 1.00 | 53.22 |
| | 451 | OD1 | ASN | 69 | 135.478 | 13.271 | 41.467 | 1.00 | 52.67 |
| | 452 | ND2 | ASN | 69 | 137.460 | 12.224 | 41.326 | 1.00 | 60.05 |
| 45 | 453 | H | ASN | 69 | 135.750 | 12.874 | 38.043 | 1.00 | 25.00 |
| | 454 | 1HD2 | ASN | 69 | 137.165 | 11.608 | 42.027 | 1.00 | 25.00 |
| | 455 | 2HD2 | ASN | 69 | 138.335 | 12.185 | 40.893 | 1.00 | 25.00 |
| | 456 | N | LEU | 70 | 136.884 | 15.813 | 37.140 | 1.00 | 26.00 |
| | 457 | CA | LEU | 70 | 137.327 | 16.958 | 36.358 | 1.00 | 27.21 |
| 50 | 458 | C | LEU | 70 | 136.135 | 17.867 | 36.053 | 1.00 | 29.79 |
| | 459 | O | LEU | 70 | 136.192 | 19.076 | 36.287 | 1.00 | 27.18 |
| | 460 | CB | LEU | 70 | 137.990 | 16.498 | 35.058 | 1.00 | 23.13 |

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|----|-----|-----|-----|----|---------|--------|--------|------|-------|
| | 461 | CG | LEU | 70 | 138.417 | 17.624 | 34.109 | 1.00 | 30.77 |
| | 462 | CD1 | LEU | 70 | 139.366 | 18.580 | 34.821 | 1.00 | 21.76 |
| | 463 | CD2 | LEU | 70 | 139.062 | 17.045 | 32.860 | 1.00 | 27.07 |
| | 464 | H | LEU | 70 | 136.995 | 14.908 | 36.777 | 1.00 | 25.00 |
| 5 | 465 | N | ILE | 71 | 135.053 | 17.272 | 35.553 | 1.00 | 30.05 |
| | 466 | CA | ILE | 71 | 133.840 | 18.012 | 35.217 | 1.00 | 24.54 |
| | 467 | C | ILE | 71 | 133.221 | 18.663 | 36.456 | 1.00 | 23.02 |
| | 468 | O | ILE | 71 | 132.849 | 19.839 | 36.429 | 1.00 | 23.20 |
| | 469 | CB | ILE | 71 | 132.809 | 17.095 | 34.516 | 1.00 | 26.68 |
| 10 | 470 | CG1 | ILE | 71 | 133.338 | 16.693 | 33.136 | 1.00 | 25.05 |
| | 471 | CG2 | ILE | 71 | 131.459 | 17.795 | 34.383 | 1.00 | 23.87 |
| | 472 | CD1 | ILE | 71 | 132.442 | 15.736 | 32.400 | 1.00 | 27.35 |
| | 473 | H | ILE | 71 | 135.073 | 16.300 | 35.409 | 1.00 | 25.00 |
| | 474 | N | ASP | 72 | 133.140 | 17.910 | 37.546 | 1.00 | 19.38 |
| 15 | 475 | CA | ASP | 72 | 132.585 | 18.429 | 38.789 | 1.00 | 22.68 |
| | 476 | C | ASP | 72 | 133.376 | 19.657 | 39.266 | 1.00 | 25.06 |
| | 477 | O | ASP | 72 | 132.784 | 20.680 | 39.626 | 1.00 | 24.92 |
| | 478 | CB | ASP | 72 | 132.593 | 17.335 | 39.861 | 1.00 | 23.74 |
| | 479 | CG | ASP | 72 | 131.900 | 17.760 | 41.147 | 1.00 | 27.65 |
| 20 | 480 | OD1 | ASP | 72 | 130.953 | 18.575 | 41.086 | 1.00 | 29.89 |
| | 481 | OD2 | ASP | 72 | 132.303 | 17.268 | 42.223 | 1.00 | 30.37 |
| | 482 | H | ASP | 72 | 133.459 | 16.986 | 37.512 | 1.00 | 25.00 |
| | 483 | N | ILE | 73 | 134.705 | 19.565 | 39.228 | 1.00 | 26.02 |
| | 484 | CA | ILE | 73 | 135.589 | 20.656 | 39.654 | 1.00 | 21.86 |
| 25 | 485 | C | ILE | 73 | 135.431 | 21.918 | 38.797 | 1.00 | 23.60 |
| | 486 | O | ILE | 73 | 135.270 | 23.019 | 39.329 | 1.00 | 25.70 |
| | 487 | CB | ILE | 73 | 137.075 | 20.198 | 39.671 | 1.00 | 20.21 |
| | 488 | CG1 | ILE | 73 | 137.245 | 19.066 | 40.684 | 1.00 | 22.84 |
| | 489 | CG2 | ILE | 73 | 137.992 | 21.351 | 40.058 | 1.00 | 17.62 |
| 30 | 490 | CD1 | ILE | 73 | 138.659 | 18.513 | 40.788 | 1.00 | 53.34 |
| | 491 | H | ILE | 73 | 135.108 | 18.732 | 38.902 | 1.00 | 25.00 |
| | 492 | N | ILE | 74 | 135.450 | 21.755 | 37.476 | 1.00 | 22.39 |
| | 493 | CA | ILE | 74 | 135.297 | 22.884 | 36.556 | 1.00 | 22.15 |
| | 494 | C | ILE | 74 | 133.955 | 23.581 | 36.784 | 1.00 | 24.59 |
| 35 | 495 | O | ILE | 74 | 133.858 | 24.807 | 36.702 | 1.00 | 29.58 |
| | 496 | CB | ILE | 74 | 135.415 | 22.426 | 35.079 | 1.00 | 24.24 |
| | 497 | CG1 | ILE | 74 | 136.835 | 21.909 | 34.811 | 1.00 | 25.85 |
| | 498 | CG2 | ILE | 74 | 135.071 | 23.571 | 34.132 | 1.00 | 19.61 |
| | 499 | CD1 | ILE | 74 | 137.054 | 21.340 | 33.420 | 1.00 | 23.74 |
| 40 | 500 | H | ILE | 74 | 135.571 | 20.851 | 37.109 | 1.00 | 25.00 |
| | 501 | N | GLU | 75 | 132.925 | 22.797 | 37.083 | 1.00 | 23.15 |
| | 502 | CA | GLU | 75 | 131.599 | 23.343 | 37.338 | 1.00 | 23.53 |
| | 503 | C | GLU | 75 | 131.548 | 24.092 | 38.658 | 1.00 | 21.84 |
| | 504 | O | GLU | 75 | 131.040 | 25.208 | 38.722 | 1.00 | 25.34 |
| 45 | 505 | CB | GLU | 75 | 130.550 | 22.237 | 37.342 | 1.00 | 26.71 |
| | 506 | CG | GLU | 75 | 130.274 | 21.647 | 35.978 | 1.00 | 30.84 |
| | 507 | CD | GLU | 75 | 129.073 | 20.720 | 35.969 | 1.00 | 36.10 |
| | 508 | OE1 | GLU | 75 | 128.644 | 20.253 | 37.051 | 1.00 | 29.89 |
| | 509 | OE2 | GLU | 75 | 128.559 | 20.460 | 34.865 | 1.00 | 31.50 |
| 50 | 510 | H | GLU | 75 | 133.056 | 21.822 | 37.122 | 1.00 | 25.00 |
| | 511 | N | ARG | 76 | 132.060 | 23.474 | 39.717 | 1.00 | 19.68 |
| | 512 | CA | ARG | 76 | 132.066 | 24.115 | 41.028 | 1.00 | 20.75 |

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|----|-----|------|------|----|---------|--------|---------|------|-------|
| | 513 | C | ARG | 76 | 132.925 | 25.385 | 41.017 | 1.00 | 22.83 |
| | 514 | O | ARG | 76 | 132.699 | 26.303 | 41.803 | 1.00 | 21.89 |
| | 515 | CB | ARG | 76 | 132.581 | 23.148 | 42.091 | 1.00 | 16.07 |
| | 516 | CG | ARG | 76 | 131.653 | 21.989 | 42.411 | 1.00 | 20.22 |
| 5 | 517 | CD | ARG | 76 | 132.331 | 21.061 | 43.395 | 1.00 | 21.08 |
| | 518 | NE | ARG | 76 | 131.498 | 19.939 | 43.819 | 1.00 | 18.53 |
| | 519 | CZ | ARG | 76 | 130.847 | 19.891 | 44.977 | 1.00 | 24.53 |
| | 520 | NH1 | ARG | 76 | 130.917 | 20.907 | 45.829 | 1.00 | 17.48 |
| | 521 | NH2 | ARG | 76 | 130.170 | 18.802 | 45.311 | 1.00 | 26.65 |
| 10 | 522 | H | ARG | 76 | 132.440 | 22.577 | 39.618 | 1.00 | 25.00 |
| | 523 | HE | ARG | 76 | 131.417 | 19.172 | 43.218 | 1.00 | 25.00 |
| | 524 | 1HH1 | ARG | 76 | 131.459 | 21.717 | 45.606 | 1.00 | 25.00 |
| | 525 | 2HH1 | ARG | 76 | 130.423 | 20.865 | 46.697 | 1.00 | 25.00 |
| | 526 | 1HH2 | ARG | 76 | 130.146 | 18.021 | 44.691 | 1.00 | 25.00 |
| 15 | 527 | 2HH2 | ARG | 76 | 129.678 | 18.766 | 46.181 | 1.00 | 25.00 |
| | 528 | N | LEU | 77 | 133.913 | 25.425 | 40.126 | 1.00 | 22.29 |
| | 529 | CA | LEU | 77 | 134.798 | 26.579 | 40.001 | 1.00 | 23.34 |
| | 530 | C | LEU | 77 | 134.156 | 27.710 | 39.193 | 1.00 | 26.64 |
| | 531 | O | LEU | 77 | 134.752 | 28.777 | 39.026 | 1.00 | 25.27 |
| 20 | 532 | CB | LEU | 77 | 136.131 | 26.167 | 39.372 | 1.00 | 18.34 |
| | 533 | CG | LEU | 77 | 137.076 | 25.352 | 40.258 | 1.00 | 18.25 |
| | 534 | CD1 | LEU | 77 | 138.266 | 24.893 | 39.443 | 1.00 | 15.60 |
| | 535 | CD2 | LEU | 77 | 137.531 | 26.182 | 41.459 | 1.00 | 17.00 |
| | 536 | H | LEU | 77 | 134.063 | 24.649 | 39.546 | 1.00 | 25.00 |
| 25 | 537 | N | GLY | 78 | 132.958 | 27.455 | 38.668 | 1.00 | 24.42 |
| | 538 | CA | GLY | 78 | 132.228 | 28.464 | 37.914 | 1.00 | 20.32 |
| | 539 | C | GLY | 78 | 132.741 | 28.807 | 36.531 | 1.00 | 20.16 |
| | 540 | O | GLY | 78 | 132.375 | 29.841 | 35.970 | 1.00 | 22.90 |
| | 541 | H | GLY | 78 | 132.553 | 26.576 | 38.793 | 1.00 | 25.00 |
| 30 | 542 | N | ILE | 79 | 133.550 | 27.927 | 335.952 | 1.00 | 22.82 |
| | 543 | CA | ILE | 79 | 134.099 | 28.170 | 34.623 | 1.00 | 24.96 |
| | 544 | C | ILE | 79 | 133.577 | 27.204 | 33.560 | 1.00 | 29.01 |
| | 545 | O | ILE | 79 | 133.991 | 27.273 | 32.398 | 1.00 | 28.78 |
| | 546 | CB | ILE | 79 | 135.646 | 28.133 | 34.635 | 1.00 | 24.44 |
| 35 | 547 | CG1 | ILE | 79 | 136.142 | 26.920 | 35.429 | 1.00 | 27.37 |
| | 548 | CG2 | ILE | 79 | 136.195 | 29.426 | 35.210 | 1.00 | 25.45 |
| | 549 | CD1 | ILE | 79 | 137.632 | 26.715 | 35.381 | 1.00 | 25.03 |
| | 550 | H | ILE | 79 | 133.782 | 27.105 | 36.435 | 1.00 | 25.00 |
| | 551 | N | SER | 80 | 132.629 | 26.347 | 33.935 | 1.00 | 27.52 |
| 40 | 552 | CA | SER | 80 | 132.079 | 25.381 | 32.986 | 1.00 | 29.32 |
| | 553 | C | SER | 80 | 131.317 | 26.012 | 31.816 | 1.00 | 31.74 |
| | 554 | O | SER | 80 | 131.187 | 25.391 | 30.761 | 1.00 | 34.93 |
| | 555 | CB | SEER | 80 | 131.205 | 24.338 | 33.694 | 1.00 | 26.24 |
| | 556 | OG | SER | 80 | 130.096 | 24.932 | 34.338 | 1.00 | 29.78 |
| 45 | 557 | H | SER | 80 | 132.308 | 26.358 | 34.857 | 1.00 | 25.00 |
| | 558 | HG | SER | 80 | 130.432 | 25.530 | 34.992 | 1.00 | 25.00 |
| | 559 | N | TYR | 81 | 130.869 | 27.258 | 31.966 | 1.00 | 25.77 |
| | 560 | CA | TYR | 81 | 130.134 | 27.914 | 30.887 | 1.00 | 23.28 |
| | 561 | C | TYR | 81 | 130.965 | 28.063 | 29.605 | 1.00 | 30.16 |
| 50 | 562 | O | TYR | 81 | 130.418 | 28.302 | 28.527 | 1.00 | 32.12 |
| | 563 | CB | TYR | 81 | 129.556 | 29.261 | 31.344 | 1.00 | 24.86 |
| | 564 | CG | TYR | 81 | 130.557 | 30.381 | 31.543 | 1.00 | 29.19 |

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|----|------|-----|-----|----|---------|--------|--------|------|-------|
| | 565 | CD1 | TYR | 81 | 131.260 | 30.519 | 32.740 | 1.00 | 27.27 |
| | 566 | CD2 | TYR | 81 | 130.768 | 31.329 | 30.545 | 1.00 | 28.18 |
| | 567 | CE1 | TYR | 81 | 132.148 | 31.575 | 32.935 | 1.00 | 29.22 |
| | 568 | CE2 | TYR | 81 | 131.649 | 32.384 | 30.729 | 1.00 | 29.85 |
| 5 | 569 | CZ | TYR | 81 | 132.336 | 32.504 | 31.923 | 1.00 | 29.78 |
| | 570 | OH | TYR | 81 | 133.220 | 33.547 | 32.084 | 1.00 | 28.93 |
| | 571 | H | TYR | 81 | 131.028 | 27.734 | 32.805 | 1.00 | 25.00 |
| | 572 | HH | TYR | 81 | 133.196 | 34.121 | 31.313 | 1.00 | 25.00 |
| | 573 | N | HIS | 82 | 132.284 | 27.904 | 29.727 | 1.00 | 32.51 |
| 10 | 574 | CA | HIS | 82 | 133.194 | 27.991 | 28.581 | 1.00 | 29.34 |
| | 575 | C | HIS | 82 | 133.237 | 26.669 | 27.828 | 1.00 | 28.19 |
| | 576 | O | HIS | 82 | 133.658 | 26.620 | 26.672 | 1.00 | 28.93 |
| | 577 | CB | HIS | 82 | 134.631 | 28.280 | 29.038 | 1.00 | 27.19 |
| | 578 | CG | HIS | 82 | 134.839 | 29.654 | 29.589 | 1.00 | 22.31 |
| 15 | 579 | ND1 | HIS | 82 | 134.702 | 30.793 | 28.825 | 1.00 | 24.56 |
| | 580 | CD2 | HIS | 82 | 135.195 | 30.071 | 30.827 | 1.00 | 20.64 |
| | 581 | CE1 | HIS | 82 | 134.964 | 31.853 | 29.568 | 1.00 | 22.72 |
| | 582 | NE2 | HIS | 82 | 135.265 | 31.442 | 30.786 | 1.00 | 23.06 |
| | 583 | H | HIS | 82 | 132.658 | 27.714 | 30.612 | 1.00 | 25.00 |
| 20 | 584 | HD1 | HIS | 82 | 134.458 | 30.815 | 27.872 | 1.00 | 25.00 |
| | 585 | HE2 | HIS | 82 | 135.465 | 32.016 | 31.549 | 1.00 | 25.00 |
| | 586 | N | PHE | 83 | 132.820 | 25.596 | 28.493 | 1.00 | 26.84 |
| | 587 | CA | PHE | 83 | 132.878 | 24.266 | 27.903 | 1.00 | 33.10 |
| | 588 | C | PHE | 83 | 131.549 | 23.521 | 27.811 | 1.00 | 36.98 |
| 25 | 589 | O | PHE | 83 | 131.511 | 22.296 | 27.973 | 1.00 | 34.23 |
| | 590 | CB | PHE | 83 | 133.895 | 23.426 | 28.683 | 1.00 | 32.26 |
| | 591 | CG | PHE | 83 | 135.171 | 24.159 | 28.985 | 1.00 | 36.23 |
| | 592 | CD1 | PHE | 83 | 136.138 | 24.336 | 27.998 | 1.00 | 36.38 |
| | 5993 | CD2 | PHE | 83 | 135.381 | 24.724 | 30.241 | 1.00 | 34.95 |
| 30 | 594 | CE1 | PHE | 83 | 137.295 | 25.067 | 28.254 | 1.00 | 36.74 |
| | 595 | CE2 | PHE | 83 | 136.533 | 25.457 | 30.509 | 1.00 | 39.63 |
| | 596 | CZ | PHE | 83 | 137.492 | 25.630 | 29.511 | 1.00 | 41.21 |
| | 597 | H | PHE | 83 | 132.457 | 25.694 | 29.394 | 1.00 | 25.00 |
| | 598 | N | GLU | 84 | 130.478 | 24.241 | 27.484 | 1.00 | 40.92 |
| 35 | 599 | CA | GLU | 84 | 129.146 | 23.641 | 27.365 | 1.00 | 46.14 |
| | 600 | C | GLU | 84 | 129.159 | 22.422 | 26.431 | 1.00 | 42.13 |
| | 601 | O | GLU | 84 | 128.753 | 21.325 | 26.819 | 1.00 | 38.24 |
| | 602 | CB | GLU | 84 | 128.128 | 24.674 | 26.851 | 1.00 | 56.77 |
| | 603 | CG | GLU | 84 | 128.042 | 25.978 | 27.660 | 1.00 | 74.38 |
| 40 | 604 | CD | GLU | 84 | 127.252 | 25.853 | 28.960 | 1.00 | 81.74 |
| | 605 | OE1 | GLU | 84 | 127.654 | 25.066 | 29.847 | 1.00 | 85.56 |
| | 606 | OE2 | GLU | 84 | 126.233 | 26.564 | 29.101 | 1.00 | 84.80 |
| | 607 | H | GLU | 84 | 130.590 | 25.203 | 27.330 | 1.00 | 25.00 |
| | 608 | N | LYS | 85 | 129.674 | 22.614 | 25.218 | 1.00 | 40.25 |
| 45 | 609 | CA | LYS | 85 | 129.740 | 21.544 | 24.224 | 1.00 | 41.41 |
| | 610 | C | LYS | 85 | 130.590 | 20.348 | 24.663 | 1.00 | 36.27 |
| | 611 | O | LYS | 85 | 130.138 | 19.204 | 24.595 | 1.00 | 35.16 |
| | 612 | CB | LYS | 85 | 130.268 | 22.085 | 22.890 | 1.00 | 46.40 |
| | 613 | CG | LYS | 85 | 130.364 | 21.025 | 21.801 | 1.00 | 58.06 |
| 50 | 614 | CD | LYS | 85 | 131.176 | 21.498 | 20.605 | 1.00 | 70.05 |
| | 615 | CE | LYS | 85 | 131.305 | 20.389 | 19.565 | 1.00 | 70.91 |
| | 616 | NZ | LYS | 85 | 132.101 | 20.809 | 18.379 | 1.00 | 79.32 |

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|----|-----|-----|-----|----|---------|--------|--------|------|-------|
| | 617 | H | LYS | 85 | 130.016 | 23.501 | 24.992 | 1.00 | 25.00 |
| | 618 | 1HZ | LYS | 85 | 133.059 | 21.080 | 18.678 | 1.00 | 25.00 |
| | 619 | 2HZ | LYS | 85 | 132.157 | 20.018 | 17.706 | 1.00 | 25.00 |
| | 620 | 3HZ | LYS | 85 | 131.636 | 21.619 | 17.922 | 1.00 | 25.00 |
| 5 | 621 | N | GLU | 86 | 131.812 | 20.620 | 25.115 | 1.00 | 37.17 |
| | 622 | CA | GLU | 86 | 132.736 | 19.573 | 25.545 | 1.00 | 35.98 |
| | 623 | C | GLU | 86 | 132.162 | 18.714 | 26.663 | 1.00 | 36.73 |
| | 624 | O | GLU | 86 | 132.156 | 17.483 | 26.571 | 1.00 | 38.05 |
| | 625 | CB | GLU | 86 | 134.077 | 20.173 | 25.990 | 1.00 | 36.51 |
| 10 | 626 | CG | GLU | 86 | 134.938 | 20.773 | 24.866 | 1.00 | 40.91 |
| | 627 | CD | GLU | 86 | 134.439 | 22.124 | 24.349 | 1.00 | 43.71 |
| | 628 | OE1 | GLU | 86 | 133.728 | 22.840 | 25.085 | 1.00 | 42.43 |
| | 629 | OE2 | GLU | 86 | 134.776 | 22.480 | 23.201 | 1.00 | 50.53 |
| | 630 | H | GLU | 86 | 132.086 | 21.551 | 25.172 | 1.00 | 25.00 |
| 15 | 631 | N | ILE | 87 | 131.666 | 19.368 | 27.708 | 1.00 | 35.80 |
| | 632 | CA | ILE | 87 | 131.092 | 18.662 | 28.845 | 1.00 | 30.66 |
| | 633 | C | ILE | 87 | 129.871 | 17.844 | 28.428 | 1.00 | 32.98 |
| | 634 | O | ILE | 87 | 129.692 | 16.711 | 28.887 | 1.00 | 32.50 |
| | 635 | CB | ILE | 87 | 130.739 | 19.640 | 29.986 | 1.00 | 30.27 |
| 20 | 636 | CG1 | ILE | 87 | 132.027 | 20.253 | 30.546 | 1.00 | 29.89 |
| | 637 | CG2 | ILE | 87 | 129.972 | 18.926 | 31.091 | 1.00 | 29.25 |
| | 638 | CD1 | ILE | 87 | 131.814 | 21.264 | 31.654 | 1.00 | 25.52 |
| | 639 | H | ILE | 87 | 131.681 | 20.348 | 27.719 | 1.00 | 25.00 |
| | 640 | N | ASP | 88 | 129.054 | 18.393 | 27.534 | 1.00 | 32.95 |
| 25 | 641 | CA | ASP | 88 | 127.870 | 17.679 | 27.070 | 1.00 | 36.69 |
| | 642 | C | ASP | 88 | 128.256 | 16.407 | 26.309 | 1.00 | 39.28 |
| | 643 | O | ASP | 88 | 127.745 | 15.324 | 26.660 | 1.00 | 40.13 |
| | 644 | CB | ASP | 88 | 126.994 | 18.573 | 26.191 | 1.00 | 40.42 |
| | 645 | CG | ASP | 88 | 125.682 | 17.901 | 25.800 | 1.00 | 49.09 |
| 30 | 646 | OD1 | ASP | 88 | 124.874 | 17.586 | 26.702 | 1.00 | 48.29 |
| | 647 | OD2 | ASP | 88 | 125.464 | 17.677 | 24.590 | 1.00 | 57.24 |
| | 648 | H | ASP | 88 | 129.245 | 19.291 | 27.185 | 1.00 | 25.00 |
| | 649 | N | GLU | 89 | 129.178 | 16.532 | 25.359 | 1.00 | 38.92 |
| | 650 | CA | GLU | 89 | 129.621 | 15.385 | 24.573 | 1.00 | 38.06 |
| 35 | 651 | C | GLU | 89 | 130.258 | 14.303 | 25.433 | 1.00 | 35.90 |
| | 652 | O | GLU | 89 | 130.077 | 13.115 | 25.168 | 1.00 | 39.91 |
| | 653 | CB | GLU | 89 | 130.572 | 15.829 | 23.466 | 1.00 | 44.42 |
| | 654 | CG | GLU | 89 | 129.871 | 16.622 | 22.379 | 1.00 | 61.34 |
| | 655 | CD | GLU | 89 | 130.822 | 17.159 | 21.333 | 1.00 | 75.40 |
| 40 | 656 | OE1 | GLU | 89 | 131.776 | 17.873 | 21.707 | 1.00 | 80.47 |
| | 657 | OE2 | GLU | 89 | 130.609 | 16.878 | 20.134 | 1.00 | 86.74 |
| | 658 | H | GLU | 89 | 129.569 | 17.416 | 25.185 | 1.00 | 25.00 |
| | 659 | N | ILE | 90 | 130.985 | 14.708 | 26.470 | 1.00 | 32.75 |
| | 660 | CA | ILE | 90 | 131.619 | 13.749 | 27.368 | 1.00 | 31.62 |
| 45 | 661 | C | ILE | 90 | 130.556 | 13.052 | 28.215 | 1.00 | 33.52 |
| | 662 | O | ILE | 90 | 130.580 | 11.830 | 28.376 | 1.00 | 35.53 |
| | 663 | CB | ILE | 90 | 132.646 | 14.427 | 28.302 | 1.00 | 31.23 |
| | 664 | CG1 | ILE | 90 | 133.815 | 14.983 | 27.485 | 1.00 | 32.25 |
| | 665 | CG2 | ILE | 90 | 133.153 | 13.431 | 29.340 | 1.00 | 23.52 |
| 50 | 666 | CD1 | ILE | 90 | 134.794 | 15.802 | 28.300 | 1.00 | 27.90 |
| | 667 | H | ILE | 90 | 131.105 | 15.670 | 26.630 | 1.00 | 25.00 |
| | 668 | N | LEU | 91 | 129.617 | 13.828 | 28.749 | 1.00 | 33.39 |

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|----|-----|------|-----|----|---------|--------|--------|------|-------|
| | 669 | CA | LEU | 91 | 128.551 | 13.266 | 29.569 | 1.00 | 33.57 |
| | 670 | C | LEU | 91 | 127.642 | 12.351 | 28.756 | 1.00 | 35.23 |
| | 671 | O | LEU | 91 | 127.145 | 11.346 | 29.269 | 1.00 | 32.55 |
| | 672 | CB | LEU | 91 | 127.741 | 14.373 | 30.244 | 1.00 | 30.86 |
| 5 | 673 | CG | LEU | 91 | 128.430 | 15.017 | 31.447 | 1.00 | 28.62 |
| | 674 | CD1 | LEU | 91 | 127.538 | 16.084 | 32.040 | 1.00 | 25.02 |
| | 675 | CD2 | LEU | 91 | 128.752 | 13.952 | 32.490 | 1.00 | 25.28 |
| | 676 | H | LEU | 91 | 129.643 | 14.796 | 28.591 | 1.00 | 25.00 |
| | 677 | N | ASP | 92 | 127.445 | 12.692 | 27.486 | 1.00 | 34.80 |
| 10 | 678 | CA | ASP | 92 | 126.620 | 11.889 | 26.595 | 1.00 | 37.65 |
| | 679 | C | ASP | 92 | 127.273 | 10.516 | 26.446 | 1.00 | 38.72 |
| | 680 | O | ASP | 92 | 126.594 | 9.490 | 26.494 | 1.00 | 41.65 |
| | 681 | CB | ASP | 92 | 126.491 | 12.569 | 25.231 | 1.00 | 44.12 |
| | 682 | CG | ASP | 92 | 125.426 | 11.931 | 24.358 | 1.00 | 48.79 |
| 15 | 683 | OD1 | ASP | 92 | 124.235 | 12.268 | 24.531 | 1.00 | 49.33 |
| | 684 | OD2 | ASP | 92 | 125.781 | 11.098 | 23.498 | 1.00 | 52.21 |
| | 685 | H | ASP | 92 | 127.856 | 13.512 | 27.149 | 1.00 | 25.00 |
| | 686 | N | GLN | 93 | 128.595 | 10.499 | 26.286 | 1.00 | 40.62 |
| | 687 | CA | GLN | 93 | 129.337 | 9.247 | 26.155 | 1.00 | 41.87 |
| 20 | 688 | C | GLN | 93 | 129.209 | 8.415 | 27.424 | 1.00 | 41.38 |
| | 689 | O | GLN | 93 | 129.038 | 7.198 | 27.356 | 1.00 | 44.29 |
| | 690 | CB | GLN | 93 | 130.817 | 9.504 | 25.883 | 1.00 | 47.84 |
| | 691 | CG | GLN | 93 | 131.124 | 10.061 | 24.511 | 1.00 | 65.26 |
| | 692 | CD | GLN | 93 | 132.618 | 10.230 | 24.286 | 1.00 | 76.60 |
| 25 | 693 | OE1 | GLN | 93 | 133.402 | 9.308 | 24.532 | 1.00 | 78.42 |
| | 694 | NE2 | GLN | 93 | 133.023 | 11.413 | 23.829 | 1.00 | 78.28 |
| | 695 | H | GLN | 93 | 129.082 | 11.351 | 26.254 | 1.00 | 25.00 |
| | 696 | 1HE2 | GLN | 93 | 133.983 | 11.522 | 23.685 | 1.00 | 25.00 |
| | 697 | 2HE2 | GLN | 93 | 132.356 | 12.108 | 23.664 | 1.00 | 25.00 |
| 30 | 698 | N | ILE | 94 | 129.302 | 9.065 | 28.580 | 1.00 | 38.08 |
| | 699 | CA | ILE | 94 | 129.186 | 8.360 | 29.851 | 1.00 | 38.56 |
| | 700 | C | ILE | 94 | 127.783 | 7.763 | 30.011 | 1.00 | 37.25 |
| | 701 | O | ILE | 94 | 127.631 | 6.623 | 30.464 | 1.00 | 40.45 |
| | 702 | CB | ILE | 94 | 129.519 | 9.284 | 31.051 | 1.00 | 38.10 |
| 35 | 703 | CG1 | ILE | 94 | 130.982 | 9.729 | 30.973 | 1.00 | 33.78 |
| | 704 | CG2 | ILE | 94 | 129.265 | 8.559 | 32.372 | 1.00 | 39.54 |
| | 705 | CD1 | ILE | 94 | 131.426 | 10.590 | 32.131 | 1.00 | 28.73 |
| | 706 | H | ILE | 94 | 129.455 | 10.035 | 28.576 | 1.00 | 25.00 |
| | 707 | N | TYR | 95 | 126.769 | 8.527 | 29.616 | 1.00 | 35.79 |
| 40 | 708 | CA | TYR | 95 | 125.383 | 8.080 | 29.702 | 1.00 | 36.92 |
| | 709 | C | TYR | 95 | 125.219 | 6.814 | 28.869 | 1.00 | 40.95 |
| | 710 | O | TYR | 95 | 124.681 | 5.812 | 29.340 | 1.00 | 39.72 |
| | 711 | CB | TYR | 95 | 124.438 | 9.170 | 29.176 | 1.00 | 31.04 |
| | 712 | CG | TYR | 95 | 122.969 | 8.799 | 29.213 | 1.00 | 35.51 |
| 45 | 713 | CD1 | TYR | 95 | 122.356 | 8.420 | 30.407 | 1.00 | 37.94 |
| | 714 | CD2 | TYR | 95 | 122.189 | 8.826 | 28.054 | 1.00 | 40.35 |
| | 715 | CE1 | TYR | 95 | 121.002 | 8.073 | 30.452 | 1.00 | 42.00 |
| | 716 | CE2 | TYR | 95 | 120.827 | 8.481 | 28.088 | 1.00 | 44.29 |
| | 717 | CZ | TYR | 95 | 120.245 | 8.107 | 29.294 | 1.00 | 43.88 |
| 50 | 718 | OH | TYR | 95 | 118.912 | 7.763 | 29.351 | 1.00 | 49.08 |
| | 719 | H | TYR | 95 | 126.959 | 9.421 | 29.265 | 1.00 | 25.00 |
| | 720 | HH | TYR | 95 | 118.668 | 7.513 | 30.254 | 1.00 | 25.00 |

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|----|-----|------|-----|-----|---------|--------|--------|------|--------|
| | 721 | N | ASN | 96 | 125.744 | 6.861 | 27.649 | 1.00 | 42.27 |
| | 722 | CA | ASN | 96 | 125.664 | 5.749 | 26.711 | 1.00 | 45.67 |
| | 723 | C | ASN | 96 | 126.430 | 4.484 | 27.088 | 1.00 | 53.96 |
| | 724 | O | ASN | 96 | 125.949 | 3.383 | 26.831 | 1.00 | 58.48 |
| 5 | 725 | CB | ASN | 96 | 126.068 | 6.215 | 25.310 | 1.00 | 41.30 |
| | 726 | CG | ASN | 96 | 125.004 | 7.072 | 24.656 | 1.00 | 45.95 |
| | 727 | OD1 | ASN | 96 | 123.922 | 6.590 | 24.339 | 1.00 | 50.40 |
| | 728 | ND2 | ASN | 96 | 125.299 | 8.349 | 24.459 | 1.00 | 47.53 |
| | 729 | H | ASN | 96 | 126.205 | 7.682 | 27.378 | 1.00 | 25.00 |
| 10 | 730 | 1HD2 | ASN | 96 | 124.616 | 8.910 | 24.040 | 1.00 | 25.00 |
| | 731 | 2HD2 | ASN | 96 | 126.172 | 8.686 | 24.743 | 1.00 | 25.00 |
| | 732 | N | GLN | 97 | 127.604 | 4.625 | 27.702 | 1.00 | 62.59 |
| | 733 | CA | GLN | 97 | 128.397 | 3.453 | 28.081 | 1.00 | 69.96 |
| | 734 | C | GLN | 97 | 127.898 | 2.701 | 29.320 | 1.00 | 74.06 |
| 15 | 735 | O | GLN | 97 | 128.255 | 1.540 | 29.521 | 1.00 | 71.27 |
| | 736 | CB | GLN | 97 | 129.885 | 3.804 | 28.219 | 1.00 | 74.21 |
| | 737 | CG | GLN | 97 | 130.227 | 4.801 | 29.315 | 1.00 | 82.49 |
| | 738 | CD | GLN | 97 | 131.723 | 5.065 | 29.415 | 1.00 | 85.73 |
| | 739 | OE1 | GLN | 97 | 132.336 | 4.837 | 30.456 | 1.00 | 88.41 |
| 20 | 740 | NE2 | GLN | 97 | 132.316 | 5.548 | 28.329 | 1.00 | 82.49 |
| | 741 | H | GLN | 97 | 127.943 | 5.524 | 27.899 | 1.00 | 25.00 |
| | 742 | 1HE2 | GLN | 97 | 133.277 | 5.711 | 28.402 | 1.00 | 25.00 |
| | 743 | 2HE2 | GLN | 97 | 131.787 | 5.714 | 27.528 | 1.00 | 25.00 |
| | 744 | N | ASN | 98 | 127.091 | 3.367 | 30.147 | 1.00 | 83.07 |
| 25 | 745 | CA | ASN | 98 | 126.517 | 2.769 | 31.360 | 1.00 | 95.02 |
| | 746 | C | ASN | 98 | 127.459 | 1.854 | 32.148 | 1.00 | 101.68 |
| | 747 | O | ASN | 98 | 127.088 | 0.737 | 32.517 | 1.00 | 106.47 |
| | 748 | CB | ASN | 98 | 125.233 | 1.997 | 31.019 | 1.00 | 98.06 |
| | 749 | CG | ASN | 98 | 124.034 | 2.902 | 30.830 | 1.00 | 100.62 |
| 30 | 750 | OD1 | ASN | 98 | 123.390 | 3.307 | 31.799 | 1.00 | 107.25 |
| | 751 | ND2 | ASN | 98 | 123.711 | 3.207 | 29.580 | 1.00 | 100.51 |
| | 752 | H | ASN | 98 | 126.876 | 4.301 | 29.938 | 1.00 | 25.00 |
| | 753 | 1HD2 | ASN | 98 | 122.944 | 3.798 | 29.449 | 1.00 | 25.00 |
| | 754 | 2HD2 | ASN | 98 | 124.241 | 2.849 | 28.838 | 1.00 | 25.00 |
| 35 | 755 | N | SER | 99 | 128.671 | 2.326 | 32.415 | 1.00 | 105.86 |
| | 756 | CA | SER | 99 | 129.649 | 1.533 | 33.153 | 1.00 | 108.38 |
| | 757 | C | SER | 999 | 129.389 | 1.528 | 34.659 | 1.00 | 109.53 |
| | 758 | O | SER | 99 | 129.054 | 2.561 | 35.243 | 1.00 | 110.32 |
| | 759 | CB | SER | 99 | 131.057 | 2.049 | 32.859 | 1.00 | 107.06 |
| 40 | 760 | OG | SER | 99 | 131.078 | 3.465 | 32.861 | 1.00 | 109.07 |
| | 761 | H | SER | 99 | 128.927 | 3.224 | 32.122 | 1.00 | 25.00 |
| | 762 | HG | SER | 99 | 130.810 | 3.805 | 33.720 | 1.00 | 25.00 |
| | 763 | N | ASN | 100 | 129.534 | 0.361 | 35.280 | 1.00 | 111.83 |
| | 764 | CA | ASN | 100 | 129.325 | 0.223 | 36.720 | 1.00 | 115.28 |
| 45 | 765 | C | ASN | 100 | 130.612 | 0.548 | 37.462 | 1.00 | 114.16 |
| | 766 | O | ASN | 100 | 131.577 | -0.213 | 37.402 | 1.00 | 114.16 |
| | 767 | CB | ASN | 100 | 128.873 | -1.195 | 37.072 | 1.00 | 117.88 |
| | 768 | CG | ASN | 100 | 127.451 | -1.473 | 36.640 | 1.00 | 122.11 |
| | 769 | OD1 | ASN | 100 | 126.518 | -0.785 | 37.056 | 1.00 | 119.89 |
| 50 | 770 | ND2 | ASN | 100 | 127.274 | -2.485 | 35.799 | 1.00 | 124.85 |
| | 771 | H | ASN | 100 | 129.794 | -0.423 | 34.757 | 1.00 | 25.00 |
| | 772 | 1HD2 | ASN | 100 | 126.354 | -2.663 | 35.510 | 1.00 | 25.00 |

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|----|-----|------|-----|-----|---------|---------|--------|------------|
| | 773 | 2HD2 | ASN | 100 | 128.048 | -3.001 | 35.500 | 1.00 25.00 |
| | 774 | N | CYS | 101 | 130.622 | 1.678 | 38.162 | 1.00112.97 |
| | 775 | CA | CYS | 101 | 131.804 | 2.103 | 38.902 | 1.00109.49 |
| 5 | 776 | C | CYS | 101 | 132.046 | 1.309 | 40.184 | 1.00104.47 |
| | 777 | O | CYS | 101 | 133.178 | 1.226 | 40.662 | 1.00107.64 |
| | 778 | CB | CYS | 101 | 131.735 | 3.593 | 39.218 | 1.00112.66 |
| | 779 | SG | CYS | 101 | 133.273 | 4.224 | 39.908 | 1.00125.35 |
| | 780 | H | CYS | 101 | 129.822 | 2.244 | 38.153 | 1.00 25.00 |
| | 781 | N | ASN | 102 | 130.976 | 0.765 | 40.756 | 1.00 95.01 |
| 10 | 782 | CA | ASN | 102 | 131.043 | -0.0488 | 41.975 | 1.00 88.33 |
| | 783 | C | ASN | 102 | 131.235 | 0.673 | 43.315 | 1.00 78.73 |
| | 784 | O | ASN | 102 | 131.005 | 0.074 | 44.367 | 1.00 78.57 |
| | 785 | CB | ASN | 102 | 132.071 | -1.182 | 41.831 | 1.00 94.60 |
| | 786 | CG | ASN | 102 | 131.727 | -2.147 | 40.704 | 1.00 99.33 |
| 15 | 787 | OD1 | ASN | 102 | 130.667 | -2.774 | 40.706 | 1.00 97.79 |
| | 788 | ND2 | ASN | 102 | 132.618 | -2.256 | 39.727 | 1.00103.54 |
| | 789 | H | ASN | 102 | 130.102 | 0.912 | 40.350 | 1.00 25.00 |
| | 790 | 1HD2 | ASN | 102 | 132.412 | -2.867 | 38.993 | 1.00 25.00 |
| | 791 | 2HD2 | ASN | 102 | 133.439 | -1.721 | 39.766 | 1.00 25.00 |
| 20 | 792 | N | ASP | 103 | 131.684 | 1.926 | 43.301 | 1.00 65.57 |
| | 793 | CA | ASP | 103 | 131.845 | 2.657 | 44.560 | 1.00 56.22 |
| | 794 | C | ASP | 103 | 130.870 | 3.833 | 44.638 | 1.00 46.49 |
| | 795 | O | ASP | 103 | 130.659 | 4.550 | 43.657 | 1.00 41.71 |
| | 796 | CB | ASP | 103 | 133.296 | 3.102 | 44.796 | 1.00 56.91 |
| 25 | 797 | CG | ASP | 103 | 133.767 | 4.133 | 43.802 | 1.00 64.49 |
| | 798 | OD1 | ASP | 103 | 134.215 | 3.735 | 42.707 | 1.00 74.22 |
| | 799 | OD2 | ASP | 103 | 133.707 | 5.339 | 44.124 | 1.00 67.65 |
| | 800 | H | ASP | 103 | 131.912 | 2.367 | 42.461 | 1.00 25.00 |
| | 801 | N | LEU | 104 | 130.281 | 4.015 | 45.816 | 1.00 38.89 |
| 30 | 802 | CA | LEU | 104 | 129.291 | 5.060 | 46.071 | 1.00 36.92 |
| | 803 | C | LEU | 104 | 129.672 | 6.457 | 45.591 | 1.00 36.45 |
| | 804 | O | LEU | 104 | 128.898 | 7.109 | 44.895 | 1.00 35.19 |
| | 805 | CB | LEU | 104 | 128.943 | 5.092 | 47.561 | 1.00 33.67 |
| | 806 | CG | LEU | 104 | 127.824 | 6.031 | 48.011 | 1.00 36.34 |
| 35 | 807 | CD1 | LEU | 104 | 126.538 | 5.713 | 47.269 | 1.00 35.38 |
| | 808 | CD2 | LEU | 104 | 127.622 | 5.893 | 49.510 | 1.00 35.29 |
| | 809 | H | LEU | 104 | 130.509 | 3.401 | 46.542 | 1.00 25.00 |
| | 810 | N | CYS | 105 | 130.872 | 6.895 | 45.951 | 1.00 36.36 |
| | 811 | CA | CYS | 105 | 131.376 | 8.212 | 45.581 | 1.00 35.11 |
| 40 | 812 | C | CYS | 105 | 131.220 | 8.537 | 44.092 | 1.00 34.06 |
| | 813 | O | CYS | 105 | 130.596 | 9.536 | 43.725 | 1.00 37.28 |
| | 814 | CB | CYS | 105 | 132.847 | 8.325 | 45.993 | 1.00 35.03 |
| | 815 | SG | CYS | 105 | 133.614 | 9.885 | 45.573 | 1.00 53.55 |
| | 816 | H | CYS | 105 | 131.437 | 6.307 | 46.484 | 1.00 25.00 |
| 45 | 817 | N | THR | 106 | 131.761 | 7.679 | 43.236 | 1.00 30.74 |
| | 818 | CA | THR | 106 | 131.697 | 7.890 | 41.797 | 1.00 28.00 |
| | 819 | C | THR | 106 | 130.301 | 7.663 | 41.227 | 1.00 25.73 |
| | 820 | O | THR | 106 | 129.870 | 8.396 | 40.339 | 1.00 28.92 |
| | 821 | CB | THR | 106 | 132.714 | 7.000 | 41.074 | 1.00 33.61 |
| 50 | 822 | OG1 | THR | 106 | 134.000 | 7.172 | 41.684 | 1.00 38.24 |
| | 823 | CG2 | THR | 106 | 132.807 | 7.369 | 39.598 | 1.00 30.78 |
| | 824 | H | THR | 106 | 132.208 | 6.874 | 43.564 | 1.00 25.00 |

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|----|-----|------|-----|-----|---------|--------|--------|------|-------|
| | 825 | HG1 | THR | 106 | 134.270 | 8.093 | 41.602 | 1.00 | 25.00 |
| | 826 | N | SER | 107 | 129.592 | 6.670 | 41.751 | 1.00 | 23.29 |
| | 827 | CA | SER | 107 | 128.237 | 6.371 | 41.294 | 1.00 | 27.37 |
| | 828 | C | SER | 107 | 127.268 | 7.540 | 41.539 | 1.00 | 25.50 |
| 5 | 829 | O | SER | 107 | 126.518 | 7.932 | 40.643 | 1.00 | 25.99 |
| | 830 | CB | SER | 107 | 127.721 | 5.101 | 41.978 | 1.00 | 26.16 |
| | 831 | OG | SER | 107 | 128.552 | 3.993 | 41.676 | 1.00 | 34.57 |
| | 832 | H | SER | 107 | 129.981 | 6.113 | 42.456 | 1.00 | 25.00 |
| | 833 | HG | SER | 107 | 128.501 | 3.864 | 40.726 | 1.00 | 25.00 |
| 10 | 834 | N | ALA | 108 | 127.298 | 8.096 | 42.749 | 1.00 | 23.90 |
| | 835 | CA | ALA | 108 | 126.441 | 9.219 | 43.121 | 1.00 | 23.63 |
| | 836 | C | ALA | 108 | 126.779 | 10.466 | 42.307 | 1.00 | 25.62 |
| | 837 | O | ALA | 108 | 125.887 | 11.189 | 41.861 | 1.00 | 27.88 |
| | 838 | CB | ALA | 108 | 126.566 | 9.509 | 44.608 | 1.00 | 18.25 |
| 15 | 839 | H | ALA | 108 | 127.913 | 7.734 | 43.418 | 1.00 | 25.00 |
| | 840 | N | LEU | 109 | 128.069 | 10.709 | 42.099 | 1.00 | 21.86 |
| | 841 | CA | LEU | 109 | 128.493 | 11.861 | 41.322 | 1.00 | 21.96 |
| | 842 | C | LEU | 109 | 128.009 | 11.704 | 39.881 | 1.00 | 25.59 |
| | 843 | O | LEU | 109 | 127.458 | 12.640 | 39.297 | 1.00 | 26.33 |
| 20 | 844 | CB | LEU | 109 | 130.017 | 12.002 | 41.359 | 1.00 | 21.29 |
| | 845 | CG | LEU | 109 | 130.611 | 13.161 | 40.550 | 1.00 | 23.03 |
| | 846 | CD1 | LEU | 109 | 129.969 | 14.480 | 40.962 | 1.00 | 15.35 |
| | 847 | CD2 | LEU | 109 | 132.111 | 13.210 | 40.751 | 1.00 | 17.60 |
| | 848 | H | LEU | 109 | 128.742 | 10.101 | 42.475 | 1.00 | 25.00 |
| 25 | 849 | N | GLN | 110 | 128.205 | 10.509 | 39.325 | 1.00 | 27.12 |
| | 850 | CA | GLN | 110 | 127.796 | 10.199 | 37.954 | 1.00 | 28.41 |
| | 851 | C | GLN | 110 | 126.302 | 10.449 | 37.803 | 1.00 | 24.05 |
| | 852 | O | GLN | 110 | 125.849 | 11.049 | 36.825 | 1.00 | 23.84 |
| | 853 | CB | GLN | 110 | 128.098 | 8.732 | 37.632 | 1.00 | 26.80 |
| 30 | 854 | CG | GLN | 110 | 127.790 | 8.333 | 36.197 | 1.00 | 34.89 |
| | 855 | CD | GLN | 110 | 127.942 | 6.843 | 35.947 | 1.00 | 37.60 |
| | 856 | OE1 | GLN | 110 | 128.418 | 6.098 | 36.804 | 1.00 | 43.99 |
| | 857 | NE2 | GLN | 110 | 127.538 | 6.401 | 34.765 | 1.00 | 38.91 |
| | 858 | H | GLN | 110 | 128.641 | 9.810 | 39.852 | 1.00 | 25.00 |
| 35 | 859 | 1HE2 | GLN | 110 | 127.636 | 5.440 | 34.604 | 1.00 | 25.00 |
| | 860 | 2HE2 | GLN | 110 | 127.167 | 7.030 | 34.117 | 1.00 | 25.00 |
| | 861 | N | PHE | 111 | 125.543 | 9.970 | 38.779 | 1.00 | 20.86 |
| | 862 | CA | PHE | 111 | 124.104 | 10.140 | 38.783 | 1.00 | 24.95 |
| | 863 | C | PHE | 111 | 123.760 | 11.633 | 38.792 | 1.00 | 24.87 |
| 40 | 864 | O | PHE | 111 | 123.037 | 12.113 | 37.917 | 1.00 | 27.29 |
| | 865 | CB | PHE | 111 | 123.511 | 9.442 | 40.008 | 1.00 | 21.47 |
| | 866 | CG | PHE | 111 | 122.019 | 9.568 | 40.120 | 1.00 | 28.99 |
| | 867 | CD1 | PHE | 111 | 121.183 | 8.649 | 39.494 | 1.00 | 24.39 |
| | 868 | CD2 | PHE | 111 | 121.448 | 10.600 | 40.865 | 1.00 | 26.46 |
| 45 | 869 | CE1 | PHE | 111 | 119.799 | 8.753 | 39.610 | 1.00 | 26.64 |
| | 870 | CE2 | PHE | 111 | 120.072 | 10.713 | 40.985 | 1.00 | 25.60 |
| | 871 | CZ | PHE | 111 | 119.243 | 9.787 | 40.356 | 1.00 | 30.12 |
| | 872 | H | PHE | 111 | 125.966 | 9.482 | 39.513 | 1.00 | 25.00 |
| | 873 | N | ARG | 112 | 124.323 | 12.372 | 39.747 | 1.00 | 23.80 |
| 50 | 874 | CA | ARG | 112 | 124.055 | 13.802 | 39.858 | 1.00 | 18.05 |
| | 875 | C | ARG | 112 | 124.384 | 14.598 | 38.601 | 1.00 | 22.05 |
| | 876 | O | ARG | 112 | 123.539 | 15.341 | 38.103 | 1.00 | 28.69 |

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|----|-----|------|------|-----|---------|--------|--------|------|-------|
| | 877 | CB | ARG | 112 | 124.771 | 14.417 | 41.066 | 1.00 | 18.30 |
| | 878 | CG | ARG | 112 | 124.503 | 15.911 | 41.209 | 1.00 | 16.54 |
| | 879 | CD | ARG | 112 | 125.077 | 16.519 | 42.479 | 1.00 | 17.13 |
| | 880 | NE | ARG | 112 | 126.540 | 16.520 | 42.517 | 1.00 | 19.87 |
| 5 | 881 | CZ | ARG | 112 | 127.323 | 17.379 | 41.866 | 1.00 | 22.23 |
| | 882 | NH1 | ARG | 112 | 126.808 | 18.328 | 41.099 | 1.00 | 19.31 |
| | 883 | NH2 | ARG | 112 | 128.636 | 17.311 | 42.012 | 1.00 | 25.31 |
| | 884 | H | ARG | 112 | 124.928 | 11.945 | 40.387 | 1.00 | 25.00 |
| | 885 | HE | ARG | 112 | 126.982 | 15.846 | 43.063 | 1.00 | 25.00 |
| 10 | 886 | 1HH1 | ARG | 112 | 125.815 | 18.407 | 40.998 | 1.00 | 25.00 |
| | 887 | 2HH1 | ARG | 112 | 127.408 | 18.960 | 40.612 | 1.00 | 25.00 |
| | 888 | 1HH2 | ARG | 112 | 129.037 | 16.615 | 42.608 | 1.00 | 25.00 |
| | 889 | 2HH2 | ARG | 112 | 129.219 | 17.950 | 41.520 | 1.00 | 25.00 |
| | 890 | N | LEU | 113 | 125.596 | 14.445 | 38.077 | 1.00 | 22.19 |
| 15 | 891 | CA | LEU | 113 | 125.994 | 15.192 | 36.883 | 1.00 | 23.19 |
| | 892 | C | LEU | 113 | 125.112 | 14.907 | 35.665 | 1.00 | 27.49 |
| | 893 | O | LEU | 113 | 124.752 | 15.828 | 34.921 | 1.00 | 24.19 |
| | 894 | CB | LEU | 113 | 127.465 | 14.937 | 36.532 | 1.00 | 26.29 |
| | 895 | CG | LEU | 113 | 128.547 | 15.323 | 37.546 | 1.00 | 28.48 |
| 20 | 896 | CD1 | LEEU | 113 | 129.911 | 15.110 | 36.905 | 1.00 | 21.83 |
| | 897 | CD2 | LEU | 113 | 128.391 | 16.772 | 37.993 | 1.00 | 17.87 |
| | 898 | H | LEU | 113 | 126.225 | 13.821 | 38.492 | 1.00 | 25.00 |
| | 899 | N | LEU | 114 | 124.776 | 13.638 | 35.451 | 1.00 | 24.90 |
| | 900 | CA | LEU | 114 | 123.932 | 13.268 | 34.321 | 1.00 | 25.28 |
| 25 | 901 | C | LEU | 114 | 122.537 | 13.867 | 34.485 | 1.00 | 23.09 |
| | 902 | O | LEU | 114 | 122.038 | 14.534 | 33.580 | 1.00 | 26.40 |
| | 903 | CB | LEU | 114 | 123.866 | 11.746 | 34.168 | 1.00 | 23.58 |
| | 904 | CG | LEU | 114 | 125.167 | 11.101 | 33.671 | 1.00 | 25.79 |
| | 905 | CD1 | LEU | 114 | 125.043 | 9.591 | 33.660 | 1.00 | 24.20 |
| 30 | 906 | CD2 | LEU | 114 | 125.504 | 11.607 | 32.280 | 1.00 | 23.62 |
| | 907 | H | LEU | 114 | 125.095 | 12.937 | 36.062 | 1.00 | 25.00 |
| | 908 | N | ARG | 115 | 121.948 | 13.694 | 35.665 | 1.00 | 23.30 |
| | 909 | CA | ARG | 115 | 120.620 | 14.228 | 35.955 | 1.00 | 21.07 |
| | 910 | C | ARG | 115 | 120.551 | 15.748 | 35.787 | 1.00 | 26.37 |
| 35 | 911 | O | ARG | 115 | 119.628 | 16.267 | 35.148 | 1.00 | 26.34 |
| | 912 | CB | ARG | 115 | 120.178 | 13.844 | 37.372 | 1.00 | 20.95 |
| | 913 | CG | ARG | 115 | 119.749 | 12.394 | 37.528 | 1.00 | 21.24 |
| | 914 | CD | ARG | 115 | 118.588 | 12.057 | 36.595 | 1.00 | 24.51 |
| | 915 | NE | ARG | 115 | 118.086 | 10.702 | 36.813 | 1.00 | 20.45 |
| 40 | 916 | CZ | ARG | 115 | 117.090 | 10.394 | 37.639 | 1.00 | 25.55 |
| | 917 | NH1 | ARG | 115 | 116.475 | 11.347 | 38.327 | 1.00 | 26.55 |
| | 918 | NH2 | ARG | 115 | 116.729 | 9.128 | 37.807 | 1.00 | 21.55 |
| | 919 | H | ARG | 115 | 122.416 | 13.187 | 36.361 | 1.00 | 25.00 |
| | 920 | HE | ARG | 115 | 118.508 | 9.978 | 36.314 | 1.00 | 25.00 |
| 45 | 921 | 1HH1 | ARG | 115 | 116.757 | 12.300 | 38.232 | 1.00 | 25.00 |
| | 922 | 2HH1 | ARG | 115 | 115.725 | 11.114 | 38.942 | 1.00 | 25.00 |
| | 923 | 1HH2 | ARG | 115 | 117.205 | 8.402 | 37.314 | 1.00 | 25.00 |
| | 924 | 2HH2 | ARG | 115 | 115.980 | 8.901 | 38.425 | 1.00 | 25.00 |
| | 925 | N | GLN | 116 | 121.537 | 16.458 | 36.333 | 1.00 | 24.98 |
| 50 | 926 | CA | GLN | 116 | 121.573 | 17.917 | 36.235 | 1.00 | 21.36 |
| | 927 | C | GLN | 116 | 121.696 | 18.366 | 34.792 | 1.00 | 23.11 |
| | 928 | O | GLN | 116 | 121.331 | 19.491 | 34.450 | 1.00 | 20.94 |

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|----|-----|------|-----|-----|---------|--------|--------|------|-------|
| | 929 | CB | GLN | 116 | 122.718 | 18.501 | 37.066 | 1.00 | 21.35 |
| | 930 | CG | GLN | 116 | 122.536 | 18.322 | 38.561 | 1.00 | 24.02 |
| | 931 | CD | GLN | 116 | 123.594 | 19.035 | 39.371 | 1.00 | 23.65 |
| 5 | 932 | OE1 | GLN | 116 | 123.278 | 19.835 | 40.252 | 1.00 | 30.06 |
| | 933 | NE2 | GLN | 116 | 124.855 | 18.744 | 39.088 | 1.00 | 21.53 |
| | 934 | H | GLN | 116 | 122.246 | 15.983 | 36.814 | 1.00 | 25.00 |
| | 935 | 1HE2 | GLN | 116 | 125.538 | 19.210 | 39.609 | 1.00 | 25.00 |
| | 936 | 2HE2 | GLN | 116 | 125.046 | 18.089 | 38.391 | 1.00 | 25.00 |
| 10 | 937 | N | HIS | 117 | 122.232 | 17.490 | 33.950 | 1.00 | 21.29 |
| | 938 | CA | HIS | 117 | 122.381 | 17.804 | 32.537 | 1.00 | 21.02 |
| | 939 | C | HIS | 117 | 121.264 | 17.235 | 31.666 | 1.00 | 23.62 |
| | 940 | O | HIS | 117 | 121.389 | 17.192 | 30.445 | 1.00 | 22.85 |
| | 941 | CB | HIS | 117 | 123.755 | 17.366 | 32.031 | 1.00 | 23.58 |
| | 942 | CG | HIS | 117 | 124.863 | 18.267 | 32.475 | 1.00 | 27.17 |
| 15 | 943 | ND1 | HIS | 117 | 125.477 | 19.165 | 31.628 | 1.00 | 28.70 |
| | 944 | CD2 | HIS | 117 | 125.421 | 18.456 | 33.693 | 1.00 | 26.70 |
| | 945 | CE1 | HIS | 117 | 126.361 | 19.874 | 32.307 | 1.00 | 25.66 |
| | 946 | NE2 | HIS | 117 | 126.346 | 19.464 | 33.562 | 1.00 | 29.17 |
| | 947 | H | HIS | 117 | 122.526 | 16.612 | 34.277 | 1.00 | 25.00 |
| 20 | 948 | HD1 | HIS | 117 | 125.301 | 19.252 | 30.671 | 1.00 | 25.00 |
| | 949 | HE2 | HIS | 117 | 126.861 | 19.825 | 34.298 | 1.00 | 25.00 |
| | 950 | N | GLY | 118 | 120.183 | 16.784 | 32.301 | 1.00 | 24.12 |
| | 951 | CA | GLY | 118 | 119.050 | 16.258 | 31.562 | 1.00 | 25.68 |
| | 952 | C | GLY | 118 | 119.037 | 14.786 | 31.193 | 1.00 | 30.13 |
| 25 | 953 | O | GLY | 118 | 118.028 | 14.303 | 30.676 | 1.00 | 35.12 |
| | 954 | H | GLY | 118 | 120.143 | 16.804 | 33.279 | 1.00 | 25.00 |
| | 955 | N | PHE | 119 | 120.130 | 14.068 | 31.432 | 1.00 | 29.49 |
| | 956 | CA | PHE | 119 | 120.184 | 12.644 | 31.102 | 1.00 | 26.30 |
| | 957 | C | PHE | 119 | 119.435 | 11.867 | 32.172 | 1.00 | 28.96 |
| 30 | 958 | O | PHE | 119 | 119.836 | 11.861 | 33.337 | 1.00 | 25.84 |
| | 959 | CB | PHE | 119 | 121.633 | 12.156 | 31.019 | 1.00 | 24.99 |
| | 960 | CG | PHE | 119 | 122.447 | 12.845 | 29.964 | 1.00 | 23.43 |
| | 961 | CD1 | PHE | 119 | 122.392 | 12.421 | 28.640 | 1.00 | 22.02 |
| | 962 | CD2 | PHE | 119 | 123.267 | 13.922 | 30.291 | 1.00 | 23.36 |
| 35 | 963 | CE1 | PHE | 119 | 123.145 | 13.063 | 27.650 | 1.00 | 26.82 |
| | 964 | CE2 | PHE | 119 | 124.023 | 14.572 | 29.312 | 1.00 | 20.73 |
| | 965 | CZ | PHE | 119 | 123.962 | 14.141 | 27.988 | 1.00 | 22.11 |
| | 966 | H | PHE | 119 | 120.902 | 14.496 | 31.856 | 1.00 | 25.00 |
| | 967 | N | ASN | 120 | 118.351 | 11.207 | 31.779 | 1.00 | 31.42 |
| 40 | 968 | CA | ASN | 120 | 117.551 | 10.447 | 32.733 | 1.00 | 36.20 |
| | 969 | C | ASN | 120 | 118.208 | 9.117 | 33.088 | 1.00 | 36.85 |
| | 970 | O | ASN | 120 | 117.727 | 8.048 | 32.707 | 1.00 | 39.49 |
| | 971 | CB | ASN | 120 | 116.126 | 10.232 | 32.200 | 1.00 | 33.41 |
| | 972 | CG | ASN | 120 | 115.142 | 9.796 | 33.286 | 1.00 | 35.58 |
| 45 | 973 | OD1 | ASN | 120 | 115.481 | 9.721 | 34.465 | 1.00 | 38.24 |
| | 974 | ND2 | ASN | 120 | 113.907 | 9.531 | 32.886 | 1.00 | 40.30 |
| | 975 | H | ASN | 120 | 118.092 | 11.226 | 30.839 | 1.00 | 25.00 |
| | 976 | 1HD2 | ASN | 120 | 113.277 | 9.246 | 33.576 | 1.00 | 25.00 |
| | 977 | 2HD2 | ASN | 120 | 113.672 | 9.626 | 31.940 | 1.00 | 25.00 |
| 50 | 978 | N | ILE | 121 | 119.347 | 9.194 | 33.770 | 1.00 | 36.98 |
| | 979 | CA | ILE | 121 | 120.054 | 7.997 | 34.192 | 1.00 | 29.59 |
| | 980 | C | ILE | 121 | 119.207 | 7.323 | 35.264 | 1.00 | 29.55 |

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|----|------|-----|-----|-----|---------|--------|---------|------|-------|
| | 981 | O | ILE | 121 | 118.647 | 7.984 | 36.134 | 1.00 | 30.63 |
| | 982 | CB | ILE | 121 | 121.478 | 8.319 | 34.745 | 1.00 | 35.93 |
| | 983 | CG1 | ILE | 121 | 122.130 | 7.046 | 35.300 | 1.00 | 34.57 |
| | 984 | CG2 | ILE | 121 | 121.419 | 9.425 | 35.7798 | 1.00 | 27.62 |
| 5 | 985 | CD1 | ILE | 121 | 123.558 | 7.221 | 35.775 | 1.00 | 37.39 |
| | 986 | H | ILE | 121 | 119.696 | 10.074 | 34.013 | 1.00 | 25.00 |
| | 987 | N | SER | 122 | 119.086 | 6.007 | 35.172 | 1.00 | 32.39 |
| | 988 | CA | SER | 122 | 118.299 | 5.245 | 36.129 | 1.00 | 27.80 |
| | 989 | C | SER | 122 | 118.912 | 5.243 | 37.526 | 1.00 | 27.11 |
| 10 | 990 | O | SER | 122 | 120.130 | 5.143 | 37.685 | 1.00 | 30.59 |
| | 991 | CB | SER | 122 | 118.145 | 3.801 | 35.642 | 1.00 | 28.47 |
| | 992 | OG | SER | 122 | 117.529 | 2.993 | 36.633 | 1.00 | 27.99 |
| | 993 | H | SER | 122 | 119.540 | 5.535 | 34.444 | 1.00 | 25.00 |
| | 994 | HG | SER | 122 | 117.442 | 2.098 | 36.275 | 1.00 | 25.00 |
| 15 | 995 | N | PRO | 123 | 118.065 | 5.325 | 38.564 | 1.00 | 27.95 |
| | 996 | CA | PRO | 123 | 118.542 | 5.323 | 39.949 | 1.00 | 27.26 |
| | 997 | C | PRO | 123 | 118.941 | 3.904 | 40.372 | 1.00 | 33.55 |
| | 998 | O | PRO | 123 | 119.325 | 3.664 | 41.521 | 1.00 | 34.51 |
| | 999 | CB | PRO | 123 | 117.323 | 5.823 | 40.723 | 1.00 | 26.86 |
| 20 | 1000 | CG | PRO | 123 | 116.184 | 5.252 | 39.938 | 1.00 | 26.05 |
| | 1001 | CD | PRO | 123 | 116.605 | 5.531 | 38.510 | 1.00 | 24.97 |
| | 1002 | N | GLU | 124 | 118.849 | 2.967 | 39.431 | 1.00 | 34.65 |
| | 1003 | CA | GLU | 124 | 119.199 | 1.569 | 39.673 | 1.00 | 42.28 |
| | 1004 | C | GLU | 124 | 120.673 | 1.441 | 40.056 | 1.00 | 39.18 |
| 25 | 1005 | O | GLU | 124 | 121.072 | 0.492 | 40.735 | 1.00 | 41.59 |
| | 1006 | CB | GLU | 124 | 118.902 | 0.732 | 38.424 | 1.00 | 48.21 |
| | 1007 | CG | GLU | 124 | 119.074 | -0.773 | 38.601 | 1.00 | 61.85 |
| | 1008 | CD | GLU | 124 | 118.112 | -1.379 | 39.615 | 1.00 | 71.29 |
| | 1009 | OE1 | GLU | 124 | 117.022 | -0.803 | 39.851 | 1.00 | 70.67 |
| 30 | 1010 | OE2 | GLU | 124 | 118.450 | -2.447 | 40.170 | 1.00 | 76.93 |
| | 1011 | H | GLU | 124 | 118.522 | 3.203 | 38.539 | 1.00 | 25.00 |
| | 1012 | N | ILE | 125 | 121.466 | 2.430 | 39.657 | 1.00 | 36.76 |
| | 1013 | CA | ILE | 125 | 122.892 | 2.458 | 39.955 | 1.00 | 35.15 |
| | 1014 | C | ILE | 125 | 123.155 | 2.401 | 41.472 | 1.00 | 35.83 |
| 35 | 1015 | O | ILE | 125 | 124.237 | 2.016 | 41.900 | 1.00 | 36.05 |
| | 1016 | CB | ILE | 125 | 123.557 | 3.718 | 39.319 | 1.00 | 33.60 |
| | 1017 | CG1 | ILE | 125 | 125.082 | 3.610 | 39.368 | 1.00 | 32.56 |
| | 1018 | CG2 | ILE | 125 | 123.087 | 4.988 | 40.017 | 1.00 | 28.43 |
| | 1019 | CD1 | ILE | 125 | 125.789 | 4.705 | 38.586 | 1.00 | 28.58 |
| 40 | 1020 | H | ILE | 125 | 121.080 | 3.169 | 39.141 | 1.00 | 25.00 |
| | 1021 | N | PHE | 126 | 122.145 | 2.733 | 42.276 | 1.00 | 33.20 |
| | 1022 | CA | PHE | 126 | 122.276 | 2.717 | 43.731 | 1.00 | 33.30 |
| | 1023 | C | PHE | 126 | 121.902 | 1.394 | 44.402 | 1.00 | 38.46 |
| | 1024 | O | PHE | 126 | 122.171 | 1.211 | 45.591 | 1.00 | 38.34 |
| 45 | 1025 | CB | PHE | 126 | 121.444 | 3.843 | 44.362 | 1.00 | 29.75 |
| | 1026 | CG | PHE | 126 | 121.937 | 5.218 | 44.030 | 1.00 | 32.61 |
| | 1027 | CD1 | PHE | 126 | 123.084 | 5.724 | 44.631 | 1.00 | 29.30 |
| | 1028 | CD2 | PHE | 126 | 121.263 | 6.007 | 43.103 | 1.00 | 33.58 |
| | 1029 | CE1 | PHE | 126 | 123.558 | 6.997 | 44.310 | 1.00 | 31.83 |
| 50 | 1030 | CE2 | PHE | 126 | 121.726 | 7.279 | 42.775 | 1.00 | 36.03 |
| | 1031 | CZ | PHE | 126 | 122.877 | 7.776 | 43.380 | 1.00 | 34.15 |
| | 1032 | H | PHE | 126 | 121.286 | 3.004 | 41.891 | 1.00 | 25.00 |

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|----|------|------|-----|-----|---------|--------|--------|------|-------|
| | 1033 | N | SER | 127 | 121.285 | 0.477 | 43.662 | 1.00 | 37.94 |
| | 1034 | CA | SER | 127 | 120.871 | -0.806 | 44.236 | 1.00 | 37.24 |
| | 1035 | C | SER | 127 | 122.012 | -1.601 | 44.855 | 1.00 | 37.05 |
| | 1036 | O | SER | 127 | 121.842 | -2.210 | 45.908 | 1.00 | 37.94 |
| 5 | 1037 | CB | SER | 127 | 120.141 | -1.658 | 43.201 | 1.00 | 34.22 |
| | 1038 | OG | SER | 127 | 118.885 | -1.087 | 42.887 | 1.00 | 44.36 |
| | 1039 | H | SER | 127 | 121.104 | 0.658 | 42.719 | 1.00 | 25.00 |
| | 1040 | HG | SER | 127 | 119.018 | -0.202 | 42.539 | 1.00 | 25.00 |
| | 1041 | N | LYS | 128 | 123.184 | -1.557 | 44.228 | 1.00 | 37.17 |
| 10 | 1042 | CA | LYS | 128 | 124.348 | -2.280 | 44.737 | 1.00 | 39.88 |
| | 1043 | C | LYS | 128 | 124.840 | -1.783 | 46.097 | 1.00 | 42.69 |
| | 1044 | O | LYS | 128 | 125.690 | -2.417 | 46.720 | 1.00 | 48.65 |
| | 1045 | CB | LYS | 128 | 125.492 | -2.257 | 43.715 | 1.00 | 39.92 |
| | 1046 | CG | LYS | 128 | 125.877 | -0.882 | 43.210 | 1.00 | 41.79 |
| 15 | 1047 | CD | LYS | 128 | 126.864 | -0.983 | 42.061 | 1.00 | 45.38 |
| | 1048 | CE | LYS | 128 | 127.112 | 0.380 | 41.430 | 1.00 | 57.33 |
| | 1049 | NZ | LYS | 128 | 128.057 | 0.329 | 40.278 | 1.00 | 63.77 |
| | 1050 | H | LYS | 128 | 123.266 | -1.028 | 43.408 | 1.00 | 25.00 |
| | 1051 | 1HZ | LYS | 128 | 128.971 | -0.047 | 40.597 | 1.00 | 25.00 |
| 20 | 1052 | 2HZ | LYS | 128 | 127.667 | -0.293 | 39.541 | 1.00 | 25.00 |
| | 1053 | 3HZ | LYS | 128 | 128.187 | 1.285 | 39.892 | 1.00 | 25.00 |
| | 1054 | N | PHE | 129 | 124.305 | -0.656 | 46.556 | 1.00 | 41.03 |
| | 1055 | CA | PHE | 129 | 124.697 | -0.090 | 47.844 | 1.00 | 38.56 |
| | 1056 | C | PHE | 129 | 123.574 | -0.255 | 48.848 | 1.00 | 42.42 |
| 25 | 1057 | O | PHE | 129 | 123.617 | 0.319 | 49.940 | 1.00 | 44.74 |
| | 1058 | CB | PHE | 129 | 125.013 | 1.396 | 47.695 | 1.00 | 32.52 |
| | 1059 | CG | PHE | 129 | 125.984 | 1.691 | 46.604 | 1.00 | 28.29 |
| | 1060 | CD1 | PHE | 129 | 127.291 | 1.225 | 46.677 | 1.00 | 27.71 |
| | 1061 | CD2 | PHE | 129 | 125.585 | 2.402 | 45.481 | 1.00 | 27.23 |
| 30 | 1062 | CE1 | PHE | 129 | 128.186 | 1.461 | 45.645 | 1.00 | 27.92 |
| | 1063 | CE2 | PHE | 129 | 126.473 | 2.644 | 44.442 | 1.00 | 29.82 |
| | 1064 | CZ | PHE | 129 | 127.776 | 2.172 | 44.523 | 1.00 | 29.88 |
| | 1065 | H | PHE | 129 | 123.617 | -0.193 | 46.037 | 1.00 | 25.00 |
| | 1066 | N | GLN | 130 | 122.566 | -1.036 | 48.482 | 1.00 | 46.51 |
| 35 | 1067 | CA | GLN | 130 | 121.425 | -1.242 | 49.356 | 1.00 | 52.21 |
| | 1068 | C | GLN | 130 | 121.181 | -2.700 | 49.659 | 1.00 | 60.08 |
| | 1069 | O | GLN | 130 | 121.565 | -3.588 | 48.891 | 1.00 | 57.60 |
| | 1070 | CB | GLN | 130 | 120.173 | -0.638 | 48.736 | 1.00 | 50.11 |
| | 1071 | CG | GLN | 130 | 120.247 | 0.860 | 48.526 | 1.00 | 50.91 |
| 40 | 1072 | CD | GLN | 130 | 119.025 | 1.399 | 47.840 | 1.00 | 51.21 |
| | 1073 | OE1 | GLN | 130 | 118.339 | 0.677 | 47.117 | 1.00 | 52.53 |
| | 1074 | NE2 | GLN | 130 | 118.737 | 2.677 | 48.061 | 1.00 | 47.70 |
| | 1075 | H | GLN | 130 | 122.585 | -1.533 | 47.632 | 1.00 | 25.00 |
| | 1076 | 1HE2 | GLN | 130 | 117.922 | 2.996 | 47.623 | 1.00 | 25.00 |
| 45 | 1077 | 2HE2 | GLN | 130 | 119.296 | 3.221 | 48.627 | 1.00 | 25.00 |
| | 1078 | N | ASP | 131 | 120.531 | -2.944 | 50.790 | 1.00 | 67.42 |
| | 1079 | CA | ASP | 131 | 120.236 | -4.306 | 51.203 | 1.00 | 74.82 |
| | 1080 | C | ASP | 131 | 118.975 | -4.746 | 50.421 | 1.00 | 79.83 |
| | 1081 | O | ASP | 131 | 118.273 | -3.905 | 49.822 | 1.00 | 81.73 |
| 50 | 1082 | CB | ASP | 131 | 120.046 | -4.394 | 52.745 | 1.00 | 75.37 |
| | 1083 | CG | ASP | 131 | 118.894 | -3.558 | 53.284 | 1.00 | 79.54 |
| | 1084 | OD1 | ASP | 131 | 118.173 | -2.911 | 52.501 | 1.00 | 89.69 |

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|----|------|------|-----|------|---------|---------|--------|------|--------|
| | 1085 | OD2 | ASP | 131 | 118.707 | -3.540 | 54.511 | 1.00 | 80.32 |
| | 1086 | H | ASP | 131 | 120.203 | -2.147 | 51.259 | 1.00 | 25.00 |
| | 1087 | N | GLU | 132 | 118.671 | -6.041 | 50.521 | 1.00 | 86.92 |
| | 1088 | CA | GLU | 132 | 117.492 | -6.620 | 49.865 | 1.00 | 93.82 |
| 5 | 1089 | C | GLU | 132 | 116.183 | -5.970 | 50.310 | 1.00 | 94.42 |
| | 1090 | O | GLU | 132 | 115.084 | -6.369 | 49.910 | 1.00 | 95.34 |
| | 1091 | CB | GLU | 132 | 117.414 | -8.108 | 50.165 | 1.00 | 99.58 |
| | 1092 | CG | GLU | 132 | 118.603 | -8.893 | 49.626 | 1.00 | 110.72 |
| | 1093 | CD | GLU | 132 | 118.550 | -10.369 | 49.968 | 1.00 | 117.77 |
| 10 | 1094 | OE1 | GLU | 132 | 118.100 | -10.716 | 51.082 | 1.00 | 122.96 |
| | 1095 | OE2 | GLU | 132 | 118.962 | -11.187 | 49.117 | 1.00 | 118.79 |
| | 1096 | H | GLU | 132 | 119.347 | -6.569 | 50.930 | 1.00 | 25.00 |
| | 1097 | N | ASN | 133 | 116.318 | -4.957 | 51.145 | 1.00 | 94.58 |
| | 1098 | CA | ASN | 1333 | 115.214 | -4.208 | 51.715 | 1.00 | 92.72 |
| 15 | 1099 | C | ASN | 133 | 115.107 | -2.839 | 51.042 | 1.00 | 90.09 |
| | 1100 | O | ASN | 133 | 114.134 | -2.112 | 51.210 | 1.00 | 90.03 |
| | 1101 | CB | ASN | 133 | 115.492 | -4.043 | 53.214 | 1.00 | 99.96 |
| | 1102 | CG | ASN | 133 | 114.389 | -3.337 | 53.923 | 1.00 | 106.41 |
| | 1103 | OD1 | ASN | 133 | 113.275 | -3.847 | 54.016 | 1.00 | 108.32 |
| 20 | 1104 | ND2 | ASN | 133 | 114.683 | -2.159 | 54.447 | 1.00 | 111.37 |
| | 1105 | H | ASN | 133 | 117.175 | -4.667 | 51.437 | 1.00 | 25.00 |
| | 1106 | 1HD2 | ASN | 133 | 113.925 | -1.736 | 54.889 | 1.00 | 25.00 |
| | 1107 | 2HD2 | ASN | 133 | 115.561 | -1.741 | 54.365 | 1.00 | 25.00 |
| | 1108 | N | GLY | 134 | 116.139 | -2.501 | 50.284 | 1.00 | 84.16 |
| 25 | 1109 | CA | GLY | 134 | 116.195 | -1.224 | 49.597 | 1.00 | 77.66 |
| | 1110 | C | GLY | 134 | 116.752 | -0.121 | 50.479 | 1.00 | 73.68 |
| | 1111 | O | GLY | 134 | 116.780 | 1.040 | 50.072 | 1.00 | 72.39 |
| | 1112 | H | GLY | 134 | 116.840 | -3.192 | 50.233 | 1.00 | 25.00 |
| | 1113 | N | LYS | 135 | 117.141 | -0.462 | 51.704 | 1.00 | 70.01 |
| 30 | 1114 | CA | LYS | 135 | 117.724 | 0.524 | 52.606 | 1.00 | 61.88 |
| | 1115 | C | LYS | 135 | 119.229 | 0.556 | 52.361 | 1.00 | 58.01 |
| | 1116 | O | LYS | 135 | 119.831 | -0.473 | 52.038 | 1.00 | 52.64 |
| | 1117 | CB | LYS | 135 | 117.429 | 0.190 | 54.069 | 1.00 | 62.54 |
| | 1118 | CG | LYS | 135 | 116.279 | 0.994 | 54.661 | 1.00 | 69.58 |
| 35 | 1119 | CD | LYS | 135 | 114.935 | 0.594 | 54.062 | 1.00 | 74.13 |
| | 1120 | CE | LYS | 135 | 113.799 | 1.517 | 54.474 | 1.00 | 77.90 |
| | 1121 | NZ | LYS | 135 | 113.779 | 1.824 | 55.931 | 1.00 | 77.60 |
| | 1122 | H | LYS | 135 | 117.045 | -1.379 | 52.010 | 1.00 | 25.00 |
| | 1123 | 1HZ | LYS | 135 | 113.687 | 0.9599 | 56.499 | 1.00 | 25.00 |
| 40 | 1124 | 2HZ | LYS | 135 | 114.669 | 2.310 | 56.155 | 1.00 | 25.00 |
| | 1125 | 3HZ | LYS | 135 | 112.977 | 2.461 | 56.110 | 1.00 | 25.00 |
| | 1126 | N | PHE | 136 | 119.834 | 1.731 | 52.491 | 1.00 | 53.56 |
| | 1127 | CA | PHE | 136 | 121.268 | 1.864 | 52.261 | 1.00 | 46.60 |
| | 1128 | C | PHE | 136 | 122.075 | 1.074 | 53.275 | 1.00 | 46.58 |
| 45 | 1129 | O | PHE | 136 | 121.797 | 1.118 | 54.473 | 1.00 | 47.43 |
| | 1130 | CB | PHE | 136 | 121.686 | 3.336 | 52.270 | 1.00 | 39.21 |
| | 1131 | CG | PHE | 136 | 121.382 | 4.056 | 50.990 | 1.00 | 32.34 |
| | 1132 | CD1 | PHE | 136 | 122.171 | 3.854 | 49.863 | 1.00 | 31.37 |
| | 1133 | CD2 | PHE | 136 | 120.282 | 4.898 | 50.896 | 1.00 | 32.38 |
| 50 | 1134 | CE1 | PHE | 136 | 121.876 | 4.491 | 48.657 | 1.00 | 25.70 |
| | 1135 | CE2 | PHE | 136 | 119.976 | 5.540 | 49.701 | 1.00 | 34.62 |
| | 1136 | CZ | PHE | 136 | 120.771 | 5.330 | 48.573 | 1.00 | 28.91 |

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|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 1137 | H | PHE | 136 | 119.315 | 2.505 | 52.789 | 1.00 | 25.00 |
| | 1138 | N | LYS | 137 | 123.046 | 0.315 | 52.776 | 1.00 | 48.31 |
| | 1139 | CA | LYS | 137 | 123.910 | -0.487 | 53.629 | 1.00 | 53.52 |
| 5 | 1140 | C | LYS | 137 | 124.551 | 0.429 | 54.656 | 1.00 | 59.01 |
| | 1141 | O | LYS | 137 | 125.408 | 1.247 | 54.316 | 1.00 | 64.30 |
| | 1142 | CB | LYS | 137 | 125.007 | -1.160 | 52.801 | 1.00 | 48.57 |
| | 1143 | CG | LYS | 137 | 124.526 | -2.258 | 51.872 | 1.00 | 52.37 |
| | 1144 | CD | LYS | 137 | 125.683 | -2.796 | 51.049 | 1.00 | 56.61 |
| | 1145 | CE | LYS | 137 | 125.266 | -3.980 | 50.199 | 1.00 | 55.76 |
| 10 | 1146 | NZ | LYS | 137 | 126.388 | -4.433 | 49.330 | 1.00 | 62.73 |
| | 1147 | H | LYS | 137 | 123.197 | 0.306 | 51.808 | 1.00 | 25.00 |
| | 1148 | 1HZ | LYS | 137 | 127.197 | -4.714 | 49.920 | 1.00 | 25.00 |
| | 1149 | 2HZ | LYS | 137 | 126.077 | -5.245 | 48.758 | 1.00 | 25.00 |
| | 1150 | 3HZ | LYS | 137 | 126.670 | -3.656 | 48.699 | 1.00 | 25.00 |
| 15 | 1151 | N | GLU | 138 | 124.151 | 0.281 | 55.914 | 1.00 | 61.30 |
| | 1152 | CA | GLU | 138 | 124.688 | 1.107 | 56.991 | 1.00 | 62.65 |
| | 1153 | C | GLU | 138 | 126.219 | 1.035 | 57.078 | 1.00 | 60.08 |
| | 1154 | O | GLU | 138 | 126.855 | 1.862 | 57.732 | 1.00 | 61.14 |
| | 1155 | CB | GLU | 138 | 124.049 | 0.720 | 58.324 | 1.00 | 63.46 |
| 20 | 1156 | CG | GLU | 138 | 122.561 | 1.033 | 58.457 | 1.00 | 67.41 |
| | 1157 | CD | GLU | 138 | 122.276 | 2.499 | 58.743 | 1.00 | 68.98 |
| | 1158 | OE1 | GLU | 138 | 122.994 | 3.105 | 59.568 | 1.00 | 67.92 |
| | 1159 | OE2 | GLU | 138 | 121.317 | 3.043 | 58.154 | 1.00 | 72.44 |
| | 1160 | H | GLU | 138 | 123.462 | -0.385 | 56.115 | 1.00 | 25.00 |
| 25 | 1161 | N | SER | 139 | 126.807 | 0.062 | 56.390 | 1.00 | 54.50 |
| | 1162 | CA | SER | 139 | 128.255 | -0.105 | 56.357 | 1.00 | 54.27 |
| | 1163 | C | SER | 139 | 128.960 | 1.037 | 55.609 | 1.00 | 51.34 |
| | 1164 | O | SER | 139 | 130.144 | 1.292 | 55.828 | 1.00 | 53.27 |
| | 1165 | CB | SER | 139 | 128.600 | -1.453 | 55.722 | 1.00 | 59.61 |
| 30 | 1166 | OG | SER | 139 | 127.596 | -1.846 | 54.800 | 1.00 | 67.84 |
| | 1167 | H | SER | 139 | 126.266 | -0.582 | 55.893 | 1.00 | 25.00 |
| | 1168 | HG | SER | 139 | 127.548 | -1.203 | 54.087 | 1.00 | 25.00 |
| | 1169 | N | LEU | 140 | 128.225 | 1.714 | 54.728 | 1.00 | 46.50 |
| | 1170 | CA | LEU | 140 | 128.751 | 2.839 | 53.953 | 1.00 | 37.91 |
| 35 | 1171 | C | LEU | 140 | 128.861 | 4.092 | 54.826 | 1.00 | 33.78 |
| | 1172 | O | LEU | 140 | 129.454 | 5.090 | 54.422 | 1.00 | 30.69 |
| | 1173 | CB | LEU | 140 | 127.821 | 3.151 | 52.777 | 1.00 | 39.38 |
| | 1174 | CG | LEU | 140 | 127.643 | 2.142 | 51.639 | 1.00 | 42.09 |
| | 1175 | CD1 | LEU | 140 | 126.330 | 2.417 | 50.919 | 1.00 | 38.48 |
| 40 | 1176 | CD2 | LEU | 140 | 128.819 | 2.212 | 50.672 | 1.00 | 38.39 |
| | 1177 | H | LEU | 140 | 127.290 | 1.456 | 54.590 | 1.00 | 25.00 |
| | 1178 | N | ALA | 141 | 128.295 | 4.024 | 56.026 | 1.00 | 28.75 |
| | 1179 | CA | ALA | 141 | 128.288 | 5.141 | 56.964 | 1.00 | 29.20 |
| | 1180 | C | ALA | 141 | 129.646 | 5.737 | 57.310 | 1.00 | 30.53 |
| 45 | 1181 | O | ALA | 141 | 129.713 | 6.825 | 57.882 | 1.00 | 30.24 |
| | 1182 | CB | ALA | 141 | 127.565 | 4.742 | 58.235 | 1.00 | 28.51 |
| | 1183 | H | ALA | 141 | 127.860 | 3.193 | 56.303 | 1.00 | 25.00 |
| | 1184 | N | SER | 142 | 130.719 | 5.018 | 57.002 | 1.00 | 28.14 |
| | 1185 | CA | SER | 142 | 132.062 | 5.500 | 57.297 | 1.00 | 30.43 |
| 50 | 1186 | C | SER | 142 | 132.788 | 6.004 | 56.051 | 1.00 | 30.66 |
| | 1187 | O | SER | 142 | 133.961 | 6.371 | 56.107 | 1.00 | 39.46 |
| | 1188 | CB | SER | 142 | 132.879 | 4.409 | 58.011 | 1.00 | 30.29 |

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|----|------|-----|-----|-----|---------|--------|---------|------|-------|
| | 1189 | OG | SER | 142 | 132.790 | 3.146 | 57.358 | 1.00 | 26.69 |
| | 1190 | H | SER | 142 | 130.627 | 4.146 | 56.569 | 1.00 | 25.00 |
| | 1191 | HG | SER | 142 | 133.417 | 2.568 | 57.780 | 1.00 | 25.00 |
| | 1192 | N | ASP | 143 | 132.069 | 6.053 | 54.937 | 1.00 | 27.41 |
| 5 | 1193 | CA | ASP | 143 | 132.614 | 6.512 | 53.663 | 1.00 | 28.00 |
| | 1194 | C | ASP | 143 | 132.168 | 7.966 | 53.447 | 1.00 | 33.02 |
| | 1195 | O | ASP | 143 | 131.211 | 8.232 | 52.714 | 1.00 | 34.43 |
| | 1196 | CB | ASP | 143 | 132.085 | 5.603 | 52.540 | 1.00 | 26.21 |
| | 1197 | CG | ASP | 143 | 132.609 | 5.978 | 51.160 | 1.00 | 32.37 |
| 10 | 1198 | OD1 | ASP | 143 | 133.578 | 6.762 | 51.045 | 1.00 | 34.10 |
| | 1199 | OD2 | ASP | 143 | 132.041 | 5.465 | 50.174 | 1.00 | 37.80 |
| | 1200 | H | ASP | 143 | 131.130 | 5.790 | 54.969 | 1.00 | 25.00 |
| | 1201 | N | VAL | 144 | 132.884 | 8.906 | 54.060 | 1.00 | 31.09 |
| | 1202 | CA | VAL | 144 | 132.548 | 10.328 | 53.958 | 1.00 | 27.23 |
| 15 | 1203 | C | VAL | 144 | 132.392 | 10.873 | 52.534 | 1.00 | 27.59 |
| | 1204 | O | VAL | 144 | 131.404 | 11.545 | 52.243 | 1.00 | 25.91 |
| | 1205 | CB | VAL | 144 | 133.541 | 11.204 | 54.758 | 1.00 | 27.72 |
| | 1206 | CG1 | VAL | 144 | 133.183 | 12.684 | 54.621 | 1.00 | 21.28 |
| | 1207 | CG2 | VAL | 144 | 133.509 | 10.804 | 56.227 | 1.00 | 34.69 |
| 20 | 1208 | H | VAL | 144 | 133.643 | 8.619 | 54.609 | 1.00 | 25.00 |
| | 1209 | N | LEU | 145 | 133.344 | 10.580 | 51.649 | 1.00 | 25.30 |
| | 1210 | CA | LEU | 145 | 133.266 | 11.063 | 50.268 | 1.00 | 27.68 |
| | 1211 | C | LEU | 145 | 132.039 | 10.510 | 49.544 | 1.00 | 29.04 |
| | 1212 | O | LEU | 145 | 131.392 | 11.218 | 48.773 | 1.00 | 26.76 |
| 25 | 1213 | CB | LEU | 145 | 134.541 | 10.722 | 49.487 | 1.00 | 27.26 |
| | 1214 | CG | LEU | 145 | 135.839 | 11.375 | 49.970 | 1.00 | 29.50 |
| | 1215 | CD1 | LEU | 145 | 136.956 | 11.087 | 48.983 | 1.00 | 25.10 |
| | 1216 | CD2 | LEU | 145 | 135.648 | 12.875 | 50.113 | 1.00 | 31.66 |
| | 1217 | H | LEU | 145 | 134.098 | 10.040 | 51.931 | 1.00 | 25.00 |
| 30 | 1218 | N | GLY | 146 | 131.717 | 9.247 | 49.806 | 1.00 | 27.11 |
| | 1219 | CA | GLY | 146 | 130.552 | 8.643 | 49.185 | 1.00 | 25.43 |
| | 1220 | C | GLY | 146 | 129.288 | 9.290 | 49.726 | 1.00 | 27.86 |
| | 1221 | O | GLY | 146 | 128.373 | 9.621 | 48.968 | 1.00 | 24.45 |
| | 1222 | H | GLY | 146 | 132.255 | 8.727 | 50.431 | 1.00 | 25.00 |
| 35 | 1223 | N | LEU | 147 | 129.251 | 9.485 | 51.043 | 1.00 | 21.13 |
| | 1224 | CA | LEU | 147 | 128.114 | 10.102 | 551.712 | 1.00 | 23.48 |
| | 1225 | C | LEU | 147 | 127.867 | 11.519 | 51.202 | 1.00 | 23.64 |
| | 1226 | O | LEU | 147 | 126.722 | 11.922 | 51.002 | 1.00 | 25.30 |
| | 1227 | CB | LEU | 147 | 128.338 | 10.140 | 53.226 | 1.00 | 23.15 |
| 40 | 1228 | CG | LEU | 147 | 128.286 | 8.821 | 54.003 | 1.00 | 30.78 |
| | 1229 | CD1 | LEU | 147 | 128.667 | 9.059 | 55.455 | 1.00 | 24.16 |
| | 1230 | CD2 | LEU | 147 | 126.892 | 8.210 | 53.911 | 1.00 | 22.86 |
| | 1231 | H | LEU | 147 | 130.010 | 9.196 | 51.584 | 1.00 | 25.00 |
| | 1232 | N | LEU | 148 | 128.943 | 12.265 | 50.978 | 1.00 | 20.29 |
| 45 | 1233 | CA | LEU | 148 | 128.831 | 13.633 | 50.498 | 1.00 | 24.04 |
| | 1234 | C | LEU | 148 | 128.217 | 13.664 | 49.106 | 1.00 | 23.69 |
| | 1235 | O | LEU | 148 | 127.267 | 14.408 | 48.855 | 1.00 | 26.51 |
| | 1236 | CB | LEU | 148 | 130.198 | 14.328 | 50.506 | 1.00 | 22.43 |
| | 1237 | CG | LEU | 148 | 130.240 | 15.787 | 50.033 | 1.00 | 24.68 |
| 50 | 1238 | CD1 | LEU | 148 | 129.285 | 16.649 | 50.853 | 1.00 | 16.95 |
| | 1239 | CD2 | LEU | 148 | 131.662 | 16.314 | 50.136 | 1.00 | 19.49 |
| | 1240 | H | LEU | 148 | 129.830 | 11.885 | 51.143 | 1.00 | 25.00 |

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|----|-------|------|-----|-----|---------|--------|--------|------|-------|
| | 1241 | N | ASN | 149 | 128.742 | 12.845 | 48.203 | 1.00 | 23.38 |
| | 1242 | CA | ASN | 149 | 128.210 | 12.801 | 46.850 | 1.00 | 20.71 |
| | 1243 | C | ASN | 149 | 126.781 | 12.269 | 46.809 | 1.00 | 25.14 |
| | 1244 | O | ASN | 149 | 125.990 | 12.678 | 45.956 | 1.00 | 25.34 |
| 5 | 1245 | CB | ASN | 149 | 129.125 | 12.008 | 45.932 | 1.00 | 15.21 |
| | 1246 | CG | ASN | 149 | 130.320 | 12.817 | 45.489 | 1.00 | 19.96 |
| | 1247 | OD1 | ASN | 149 | 131.340 | 12.856 | 46.167 | 1.00 | 34.43 |
| | 1248 | ND2 | ASN | 149 | 130.185 | 13.505 | 44.369 | 1.00 | 25.72 |
| | 1249 | H | ASN | 149 | 129.509 | 12.271 | 48.444 | 1.00 | 25.00 |
| 10 | 1250 | 1HD2 | ASN | 149 | 130.969 | 14.021 | 44.090 | 1.00 | 25.00 |
| | 1251 | 2HD2 | ASN | 149 | 129.340 | 13.468 | 43.887 | 1.00 | 25.00 |
| | 1252 | N | LEU | 150 | 126.445 | 11.379 | 47.743 | 1.00 | 21.91 |
| | 1253 | CA | LEU | 150 | 125.096 | 10.829 | 47.827 | 1.00 | 24.64 |
| | 1254 | C | LEU | 150 | 124.171 | 11.938 | 48.330 | 1.00 | 22.13 |
| 15 | 1255 | O | LEU | 150 | 123.058 | 12.104 | 47.831 | 1.00 | 27.92 |
| | 1256 | CB | LEU | 150 | 125.051 | 9.630 | 48.780 | 1.00 | 17.59 |
| | 1257 | CG | LEU | 150 | 123.659 | 9.057 | 49.062 | 1.00 | 21.25 |
| | 1258 | CD1 | LEU | 150 | 123.054 | 8.510 | 47.780 | 1.00 | 18.26 |
| | 1259 | CD2 | LEU | 150 | 123.739 | 7.976 | 50.118 | 1.00 | 19.18 |
| 20 | 1260 | H | LEU | 150 | 127.125 | 11.076 | 48.382 | 1.00 | 25.00 |
| | 1261 | N | TYR | 151 | 124.652 | 12.706 | 49.301 | 1.00 | 20.18 |
| | 1262 | CA | TYR | 151 | 123.892 | 13.818 | 49.858 | 1.00 | 20.96 |
| | 1263 | C | TYR | 151 | 123.533 | 14.798 | 48.738 | 1.00 | 19.39 |
| | 1264 | O | TYR | 151 | 122.380 | 15.204 | 48.592 | 1.00 | 21.76 |
| 25 | 1265 | CB | TYR | 151 | 124.723 | 14.535 | 50.929 | 1.00 | 20.29 |
| | 1266 | CG | TYR | 151 | 124.115 | 15.828 | 51.418 | 1.00 | 22.32 |
| | 1267 | CD1 | TYR | 151 | 123.202 | 15.834 | 52.470 | 1.00 | 20.29 |
| | 1268 | CD2 | TYR | 151 | 124.432 | 17.047 | 50.811 | 1.00 | 21.17 |
| | 1269 | CE1 | TYR | 151 | 122.614 | 17.021 | 52.907 | 1.00 | 20.42 |
| 30 | 1270 | CE2 | TYR | 151 | 123.850 | 18.236 | 51.237 | 1.00 | 21.39 |
| | 1271 | CZ | TYR | 151 | 122.940 | 18.214 | 52.285 | 1.00 | 22.07 |
| | 1272 | OH | TYR | 151 | 122.337 | 19.377 | 52.696 | 1.00 | 21.54 |
| | 1273 | H | TYR | 151 | 125.542 | 12.522 | 49.655 | 1.00 | 25.00 |
| | 1274 | HH | TYR | 151 | 121.769 | 19.210 | 53.457 | 1.00 | 25.00 |
| 35 | 12775 | N | GLU | 152 | 124.532 | 15.194 | 47.959 | 1.00 | 21.41 |
| | 1276 | CA | GLU | 152 | 124.316 | 16.128 | 46.863 | 1.00 | 19.05 |
| | 1277 | C | GLU | 152 | 123.388 | 15.546 | 45.800 | 1.00 | 23.34 |
| | 1278 | O | GLU | 152 | 122.540 | 16.259 | 45.260 | 1.00 | 21.99 |
| | 1279 | CB | GLU | 152 | 125.653 | 16.544 | 46.235 | 1.00 | 23.58 |
| 40 | 1280 | CG | GLU | 152 | 126.641 | 17.236 | 47.198 | 1.00 | 23.54 |
| | 1281 | CD | GLU | 152 | 126.245 | 18.662 | 47.577 | 1.00 | 27.07 |
| | 1282 | OE1 | GLU | 152 | 125.046 | 19.009 | 47.529 | 1.00 | 30.35 |
| | 1283 | OE2 | GLU | 152 | 127.145 | 19.444 | 47.935 | 1.00 | 23.20 |
| | 1284 | H | GLU | 152 | 125.434 | 14.851 | 48.136 | 1.00 | 25.00 |
| 45 | 1285 | N | ALA | 153 | 123.530 | 14.248 | 45.526 | 1.00 | 24.42 |
| | 1286 | CA | ALA | 153 | 122.706 | 13.565 | 44.526 | 1.00 | 22.61 |
| | 1287 | C | ALA | 153 | 121.251 | 13.409 | 44.964 | 1.00 | 19.49 |
| | 1288 | O | ALA | 153 | 120.342 | 13.450 | 44.138 | 1.00 | 21.30 |
| | 1289 | CB | ALA | 153 | 123.300 | 12.203 | 44.186 | 1.00 | 21.47 |
| 50 | 1290 | H | ALA | 153 | 124.211 | 13.731 | 46.006 | 1.00 | 25.00 |
| | 1291 | N | SER | 154 | 121.026 | 13.262 | 46.264 | 1.00 | 16.33 |
| | 1292 | CA | SER | 154 | 119.672 | 13.105 | 46.776 | 1.00 | 21.77 |

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|----|------|------|-----|-----|---------|--------|---------|------|-------|
| | 1293 | C | SER | 154 | 118.822 | 14.343 | 46.464 | 1.00 | 27.62 |
| | 1294 | O | SER | 154 | 117.603 | 14.258 | 46.351 | 1.00 | 29.95 |
| | 1295 | CB | SER | 154 | 119.688 | 12.820 | 48.288 | 1.00 | 15.72 |
| | 1296 | OG | SER | 154 | 119.902 | 13.991 | 49.060 | 1.00 | 20.33 |
| 5 | 1297 | H | SER | 154 | 121.776 | 13.256 | 46.901 | 1.00 | 25.00 |
| | 1298 | HG | SER | 154 | 119.193 | 14.609 | 48.898 | 1.00 | 25.00 |
| | 1299 | N | HIS | 155 | 119.470 | 15.489 | 46.291 | 1.00 | 24.50 |
| | 1300 | CA | HIS | 155 | 118.751 | 16.720 | 46.001 | 1.00 | 20.74 |
| | 1301 | C | HIS | 155 | 118.320 | 16.907 | 44.552 | 1.00 | 22.52 |
| 10 | 1302 | O | HIS | 155 | 117.682 | 17.905 | 44.224 | 1.00 | 23.13 |
| | 1303 | CB | HIS | 155 | 119.543 | 17.929 | 46.487 | 1.00 | 19.93 |
| | 1304 | CG | HIS | 155 | 119.439 | 18.154 | 47.961 | 1.00 | 14.77 |
| | 1305 | ND1 | HIS | 155 | 120.456 | 17.843 | 48.838 | 1.00 | 20.63 |
| | 1306 | CD2 | HIS | 155 | 118.431 | 18.652 | 48.716 | 1.00 | 13.91 |
| 15 | 1307 | CE1 | HIS | 155 | 120.080 | 18.142 | 50.069 | 1.00 | 21.57 |
| | 1308 | NE2 | HIS | 155 | 118.855 | 18.634 | 50.022 | 1.00 | 17.34 |
| | 1309 | H | HIS | 155 | 120.451 | 15.494 | 46.346 | 1.00 | 25.00 |
| | 1310 | HD1 | HIS | 155 | 121.317 | 17.420 | 48.603 | 1.00 | 25.00 |
| | 1311 | HE2 | HIS | 155 | 118.336 | 18.952 | 50.793 | 1.00 | 25.00 |
| 20 | 1312 | N | VAL | 156 | 118.686 | 15.972 | 43.678 | 1.00 | 22.99 |
| | 1313 | CA | VAL | 156 | 118.283 | 16.063 | 42.276 | 1.00 | 22.09 |
| | 1314 | C | VAL | 156 | 117.265 | 14.970 | 41.940 | 1.00 | 22.99 |
| | 1315 | O | VAL | 156 | 116.954 | 14.741 | 40.768 | 1.00 | 22.80 |
| | 1316 | CB | VAL | 156 | 119.491 | 15.956 | 41.299 | 1.00 | 18.92 |
| 25 | 1317 | CG1 | VAL | 156 | 120.541 | 16.999 | 41.636 | 1.00 | 20.34 |
| | 1318 | CG2 | VAL | 156 | 120.089 | 14.560 | 41.329 | 1.00 | 20.67 |
| | 1319 | H | VAL | 156 | 119.229 | 15.207 | 43.966 | 1.00 | 25.00 |
| | 1320 | N | ARG | 157 | 116.729 | 14.317 | 42.968 | 1.00 | 19.28 |
| | 1321 | CA | ARG | 157 | 115.766 | 13.239 | 42.762 | 1.00 | 25.29 |
| 30 | 1322 | C | ARG | 157 | 114.394 | 13.708 | 42.272 | 1.00 | 26.91 |
| | 1323 | O | ARG | 157 | 113.988 | 14.850 | 42.498 | 1.00 | 27.10 |
| | 1324 | CB | ARG | 157 | 115.625 | 12.380 | 44.024 | 1.00 | 19.93 |
| | 1325 | CG | ARG | 157 | 114.831 | 13.011 | 45.1144 | 1.00 | 19.14 |
| | 1326 | CD | ARG | 157 | 114.914 | 12.156 | 46.397 | 1.00 | 20.33 |
| 35 | 1327 | NE | ARG | 157 | 114.069 | 12.674 | 47.473 | 1.00 | 30.46 |
| | 1328 | CZ | ARG | 157 | 114.373 | 13.717 | 48.242 | 1.00 | 36.78 |
| | 1329 | NH1 | ARG | 157 | 115.515 | 14.371 | 48.071 | 1.00 | 39.31 |
| | 1330 | NH2 | ARG | 157 | 113.523 | 14.119 | 49.176 | 1.00 | 36.74 |
| | 1331 | H | ARG | 157 | 116.972 | 14.566 | 43.881 | 1.00 | 25.00 |
| 40 | 1332 | HE | ARG | 157 | 113.214 | 12.230 | 47.643 | 1.00 | 25.00 |
| | 1333 | 1HH1 | ARG | 157 | 116.149 | 14.079 | 47.364 | 1.00 | 25.00 |
| | 1334 | 2HH1 | ARG | 157 | 115.736 | 15.154 | 48.652 | 1.00 | 25.00 |
| | 1335 | 1HH2 | ARG | 157 | 112.655 | 13.643 | 49.305 | 1.00 | 25.00 |
| | 1336 | 2HH2 | ARG | 157 | 113.751 | 14.905 | 49.753 | 1.00 | 25.00 |
| 45 | 1337 | N | THR | 158 | 113.709 | 12.813 | 41.569 | 1.00 | 30.13 |
| | 1338 | CA | THR | 158 | 112.385 | 13.066 | 41.015 | 1.00 | 27.65 |
| | 1339 | C | THR | 158 | 111.374 | 12.189 | 41.763 | 1.00 | 25.41 |
| | 1340 | O | THR | 158 | 111.751 | 11.413 | 42.642 | 1.00 | 23.51 |
| | 1341 | CB | THR | 158 | 112.350 | 12.703 | 39.513 | 1.00 | 24.84 |
| 50 | 1342 | OG1 | THR | 158 | 112.630 | 11.307 | 39.355 | 1.00 | 27.71 |
| | 1343 | CG2 | THR | 158 | 113.391 | 13.496 | 38.738 | 1.00 | 19.09 |
| | 1344 | H | THR | 158 | 114.102 | 11.937 | 41.427 | 1.00 | 25.00 |

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|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 1345 | HG1 | THR | 158 | 111.995 | 10.771 | 39.817 | 1.00 | 25.00 |
| | 1346 | N | HIS | 159 | 110.103 | 12.268 | 41.377 | 1.00 | 26.77 |
| | 1347 | CA | HIS | 159 | 109.051 | 11.473 | 42.016 | 1.00 | 27.30 |
| | 1348 | C | HIS | 159 | 109.196 | 9.971 | 41.741 | 1.00 | 33.58 |
| 5 | 1349 | O | HIS | 159 | 108.630 | 9.150 | 42.462 | 1.00 | 33.82 |
| | 1350 | CB | HIS | 159 | 107.663 | 11.939 | 41.557 | 1.00 | 26.01 |
| | 1351 | CG | HIS | 159 | 107.337 | 13.350 | 41.941 | 1.00 | 23.00 |
| | 1352 | ND1 | HIS | 159 | 106.999 | 13.711 | 43.226 | 1.00 | 24.86 |
| | 1353 | CD2 | HIS | 159 | 107.311 | 14.490 | 41.210 | 1.00 | 18.70 |
| 10 | 1354 | CE1 | HIS | 159 | 106.782 | 15.012 | 43.275 | 1.00 | 24.72 |
| | 1355 | NE2 | HIS | 159 | 106.966 | 15.509 | 42.064 | 1.00 | 23.55 |
| | 1356 | H | HIS | 159 | 109.879 | 12.878 | 40.646 | 1.00 | 25.00 |
| | 1357 | HD1 | HIS | 159 | 106.924 | 13.094 | 43.988 | 1.00 | 25.00 |
| | 1358 | HE2 | HIS | 159 | 106.880 | 16.460 | 41.845 | 1.00 | 25.00 |
| 15 | 1359 | N | ALA | 160 | 109.948 | 9.624 | 40.697 | 1.00 | 32.77 |
| | 1360 | CA | ALA | 160 | 110.167 | 8.229 | 40.315 | 1.00 | 31.64 |
| | 1361 | C | ALA | 160 | 111.364 | 7.581 | 41.009 | 1.00 | 36.31 |
| | 1362 | O | ALA | 160 | 111.509 | 6.361 | 41.002 | 1.00 | 37.53 |
| | 1363 | CB | ALA | 160 | 110.326 | 8.130 | 38.803 | 1.00 | 25.40 |
| 20 | 1364 | H | ALA | 160 | 110.358 | 10.319 | 40.160 | 1.00 | 25.00 |
| | 1365 | N | ASP | 161 | 112.217 | 8.401 | 41.612 | 1.00 | 40.41 |
| | 1366 | CA | ASP | 161 | 113.415 | 7.904 | 42.281 | 1.00 | 40.26 |
| | 1367 | C | ASP | 161 | 113.123 | 7.414 | 43.689 | 1.00 | 41.77 |
| | 1368 | O | ASP | 161 | 113.634 | 7.937 | 44.678 | 1.00 | 41.48 |
| 25 | 1369 | CB | ASP | 161 | 114.508 | 8.976 | 42.291 | 1.00 | 34.22 |
| | 1370 | CG | ASP | 161 | 114.959 | 9.354 | 40.898 | 1.00 | 34.94 |
| | 1371 | OD1 | ASP | 161 | 114.954 | 8.486 | 40.002 | 1.00 | 33.51 |
| | 1372 | OD2 | ASP | 161 | 115.319 | 10.532 | 40.697 | 1.00 | 32.35 |
| | 1373 | H | ASP | 161 | 112.014 | 9.350 | 41.663 | 1.00 | 25.00 |
| 30 | 1374 | N | ASP | 162 | 112.353 | 6.342 | 43.742 | 1.00 | 46.26 |
| | 1375 | CA | ASP | 162 | 111.932 | 5.726 | 44.985 | 1.00 | 46.59 |
| | 1376 | C | ASP | 162 | 113.108 | 5.156 | 45.760 | 1.00 | 44.37 |
| | 1377 | O | ASP | 162 | 113.127 | 5.172 | 46.990 | 1.00 | 37.28 |
| | 1378 | CB | ASP | 162 | 110.916 | 4.630 | 44.670 | 1.00 | 56.78 |
| 35 | 1379 | CG | ASP | 162 | 109.654 | 5.185 | 44.046 | 1.00 | 69.65 |
| | 1380 | OD1 | ASP | 162 | 108.899 | 5.870 | 44.766 | 1.00 | 67.08 |
| | 1381 | OD2 | ASP | 162 | 109.435 | 4.978 | 42.830 | 1.00 | 79.19 |
| | 1382 | H | ASP | 162 | 112.114 | 5.949 | 42.869 | 1.00 | 25.00 |
| | 1383 | N | ILE | 163 | 114.106 | 4.699 | 45.015 | 1.00 | 41.87 |
| 40 | 1384 | CA | ILE | 163 | 115.314 | 4.112 | 45.575 | 1.00 | 43.77 |
| | 1385 | C | ILE | 163 | 116.093 | 5.124 | 46.426 | 1.00 | 42.36 |
| | 1386 | O | ILE | 163 | 116.764 | 4.757 | 47.385 | 1.00 | 45.56 |
| | 1387 | CB | ILE | 163 | 116.200 | 3.561 | 44.433 | 1.00 | 47.25 |
| | 1388 | CG1 | ILE | 163 | 115.385 | 2.571 | 43.595 | 1.00 | 56.48 |
| 45 | 1389 | CG2 | ILE | 163 | 117.433 | 2.870 | 44.986 | 1.00 | 49.93 |
| | 1390 | CD1 | ILE | 163 | 116.134 | 1.994 | 42.404 | 1.00 | 60.37 |
| | 1391 | H | ILE | 163 | 114.031 | 4.781 | 44.043 | 1.00 | 25.00 |
| | 1392 | N | LEU | 164 | 115.955 | 6.404 | 46.097 | 1.00 | 37.87 |
| | 1393 | CA | LEU | 164 | 116.650 | 7.473 | 46.805 | 1.00 | 33.53 |
| 50 | 1394 | C | LEU | 164 | 115.828 | 8.132 | 47.897 | 1.00 | 32.57 |
| | 1395 | O | LEU | 164 | 116.206 | 9.192 | 48.400 | 1.00 | 36.58 |
| | 1396 | CB | LEU | 164 | 117.102 | 8.542 | 45.815 | 1.00 | 30.53 |

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|----|------|-----|-----|------|---------|--------|--------|------|-------|
| | 1397 | CG | LEU | 164 | 118.184 | 8.139 | 44.815 | 1.00 | 36.53 |
| | 1398 | CD1 | LEU | 164 | 118.416 | 9.266 | 43.820 | 1.00 | 26.74 |
| | 1399 | CD2 | LEU | 164 | 119.468 | 7.794 | 45.562 | 1.00 | 30.59 |
| 5 | 1400 | H | LEU | 164 | 115.309 | 6.641 | 45.397 | 1.00 | 25.00 |
| | 1401 | N | GLU | 165 | 114.737 | 7.489 | 48.290 | 1.00 | 32.57 |
| | 1402 | CA | GLU | 165 | 113.854 | 8.022 | 49.320 | 1.00 | 32.62 |
| | 1403 | C | GLU | 165 | 114.537 | 8.326 | 50.655 | 1.00 | 35.56 |
| | 1404 | O | GLU | 165 | 114.298 | 9.368 | 51.267 | 1.00 | 35.70 |
| 10 | 1405 | CB | GLU | 165 | 112.683 | 7.058 | 49.551 | 1.00 | 39.90 |
| | 1406 | CG | GLU | 165 | 111.645 | 7.571 | 50.549 | 1.00 | 50.03 |
| | 1407 | CD | GLU | 165 | 111.021 | 8.886 | 50.115 | 1.00 | 59.83 |
| | 1408 | OE1 | GLU | 165 | 110.492 | 8.952 | 48.983 | 1.00 | 63.90 |
| | 1409 | OE2 | GLU | 165 | 111.069 | 9.862 | 50.899 | 1.00 | 58.42 |
| | 1410 | H | GLU | 165 | 114.553 | 6.614 | 47.898 | 1.00 | 25.00 |
| 15 | 1411 | N | ASP | 166 | 115.411 | 7.431 | 51.091 | 1.00 | 37.81 |
| | 1412 | CA | ASP | 166 | 116.079 | 7.609 | 52.369 | 1.00 | 43.12 |
| | 1413 | C | ASP | 166 | 117.546 | 8.030 | 52.268 | 1.00 | 40.48 |
| | 1414 | O | ASP | 166 | 118.274 | 8.039 | 53.262 | 1.00 | 40.91 |
| | 1415 | CB | ASP | 166 | 115.899 | 6.352 | 53.234 | 1.00 | 51.99 |
| 20 | 1416 | CG | ASP | 168 | 114.532 | 6.303 | 53.902 | 1.00 | 67.29 |
| | 1417 | OD1 | ASP | 166 | 114.268 | 7.173 | 54.761 | 1.00 | 74.04 |
| | 1418 | OD2 | ASP | 166 | 113.712 | 5.423 | 53.552 | 1.00 | 74.06 |
| | 1419 | H | ASP | 166 | 115.669 | 6.693 | 50.506 | 1.00 | 25.00 |
| | 1420 | N | ALA | 167 | 117.939 | 8.459 | 51.075 | 1.00 | 34.07 |
| 25 | 1421 | CA | ALA | 167 | 119.298 | 8.902 | 50.806 | 1.00 | 30.06 |
| | 1422 | C | ALA | 167 | 119.664 | 10.182 | 51.554 | 1.00 | 33.12 |
| | 1423 | O | ALA | 167 | 120.759 | 10.292 | 52.103 | 1.00 | 34.41 |
| | 1424 | CB | ALA | 167 | 119.488 | 9.090 | 49.308 | 1.00 | 25.56 |
| | 1425 | H | ALA | 167 | 117.260 | 8.486 | 50.375 | 1.00 | 25.00 |
| 30 | 1426 | N | LEU | 168 | 118.737 | 11.134 | 51.593 | 1.00 | 34.35 |
| | 1427 | CA | LEU | 168 | 118.975 | 12.403 | 52.268 | 1.00 | 29.26 |
| | 1428 | C | LEU | 168 | 119.184 | 12.226 | 53.764 | 1.00 | 32.06 |
| | 1429 | O | LEU | 168 | 120.199 | 12.656 | 54.311 | 1.00 | 34.07 |
| | 1430 | CB | LEU | 168 | 117.820 | 13.381 | 52.024 | 1.00 | 25.73 |
| 35 | 1431 | CG | LEU | 168 | 117.980 | 14.767 | 52.671 | 1.00 | 29.40 |
| | 1432 | CD1 | LEU | 168 | 119.241 | 15.454 | 52.153 | 1.00 | 22.56 |
| | 1433 | CD2 | LEU | 168 | 116.765 | 15.635 | 52.397 | 1.00 | 28.30 |
| | 1434 | H | LEU | 168 | 117.879 | 10.944 | 51.168 | 1.00 | 25.00 |
| | 1435 | N | ALA | 169 | 118.224 | 11.593 | 54.425 | 1.00 | 32.55 |
| 40 | 1436 | CA | ALA | 169 | 118.317 | 11.372 | 55.865 | 1.00 | 37.53 |
| | 1437 | C | ALA | 169 | 119.561 | 10.552 | 56.227 | 1.00 | 37.81 |
| | 1438 | O | ALA | 169 | 120.273 | 10.873 | 57.185 | 1.00 | 38.90 |
| | 1439 | CB | ALA | 1669 | 117.058 | 10.680 | 56.370 | 1.00 | 36.88 |
| | 1440 | H | ALA | 169 | 117.444 | 11.265 | 53.938 | 1.00 | 25.00 |
| 45 | 1441 | N | PHE | 170 | 119.830 | 9.520 | 55.429 | 1.00 | 30.70 |
| | 1442 | CA | PHE | 170 | 120.976 | 8.640 | 55.635 | 1.00 | 29.14 |
| | 1443 | C | PHE | 170 | 122.296 | 9.413 | 55.592 | 1.00 | 31.93 |
| | 1444 | O | PHE | 170 | 123.046 | 9.432 | 56.573 | 1.00 | 35.80 |
| | 1445 | CB | PHE | 170 | 120.978 | 7.538 | 54.569 | 1.00 | 27.52 |
| 50 | 1446 | CG | PHE | 170 | 122.093 | 6.538 | 54.719 | 1.00 | 29.21 |
| | 1447 | CD1 | PHE | 170 | 122.055 | 5.576 | 55.722 | 1.00 | 32.25 |
| | 1448 | CD2 | PHE | 170 | 123.178 | 6.553 | 53.850 | 1.00 | 31.23 |

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|----|------|------|-----|-----|---------|--------|--------|------|-------|
| | 1449 | CE1 | PHE | 170 | 123.085 | 4.642 | 55.854 | 1.00 | 35.77 |
| | 1450 | CE2 | PHE | 170 | 124.213 | 5.624 | 53.974 | 1.00 | 28.29 |
| | 1451 | CZ | PHE | 170 | 124.166 | 4.668 | 54.977 | 1.00 | 33.63 |
| | 1452 | H | PHE | 170 | 119.237 | 9.336 | 54.671 | 1.00 | 25.00 |
| 5 | 1453 | N | SER | 171 | 122.572 | 10.054 | 54.460 | 1.00 | 29.96 |
| | 1454 | CA | SER | 171 | 123.803 | 10.817 | 54.297 | 1.00 | 23.74 |
| | 1455 | C | SER | 171 | 123.888 | 11.970 | 55.293 | 1.00 | 25.49 |
| | 1456 | O | SER | 171 | 124.951 | 12.232 | 55.845 | 1.00 | 30.00 |
| | 1457 | CB | SER | 171 | 123.927 | 11.333 | 52.860 | 1.00 | 25.16 |
| 10 | 1458 | OG | SER | 171 | 122.818 | 12.137 | 52.501 | 1.00 | 31.46 |
| | 1459 | H | SER | 171 | 121.937 | 10.029 | 53.708 | 1.00 | 25.00 |
| | 1460 | HG | SER | 171 | 122.754 | 12.902 | 53.078 | 1.00 | 25.00 |
| | 1461 | N | THR | 172 | 122.761 | 12.625 | 55.557 | 1.00 | 25.72 |
| | 1462 | CA | THR | 172 | 122.728 | 13.746 | 56.490 | 1.00 | 25.18 |
| 15 | 1463 | C | THR | 172 | 123.183 | 13.367 | 57.902 | 1.00 | 30.69 |
| | 1464 | O | THR | 172 | 124.122 | 13.961 | 58.438 | 1.00 | 29.76 |
| | 1465 | CB | THR | 172 | 121.311 | 14.390 | 56.574 | 1.00 | 24.33 |
| | 1466 | OG1 | THR | 172 | 120.958 | 14.958 | 55.307 | 1.00 | 19.73 |
| | 1467 | CG2 | THR | 172 | 121.282 | 15.499 | 57.620 | 1.00 | 16.92 |
| 20 | 1468 | H | THR | 172 | 121.932 | 12.351 | 55.113 | 1.00 | 25.00 |
| | 1469 | HG1 | THR | 172 | 120.938 | 14.264 | 54.646 | 1.00 | 25.00 |
| | 1470 | N | ILE | 173 | 122.542 | 12.363 | 58.489 | 1.00 | 34.29 |
| | 1471 | CA | ILE | 173 | 122.875 | 11.951 | 59.848 | 1.00 | 37.02 |
| | 1472 | C | ILE | 173 | 124.319 | 11.488 | 60.017 | 1.00 | 31.30 |
| 25 | 1473 | O | ILE | 173 | 124.956 | 11.777 | 61.032 | 1.00 | 34.03 |
| | 1474 | CB | ILE | 173 | 121.894 | 10.870 | 60.384 | 1.00 | 42.89 |
| | 1475 | CG1 | ILE | 173 | 122.082 | 10.702 | 61.893 | 1.00 | 46.46 |
| | 1476 | CG2 | ILE | 173 | 122.115 | 9.539 | 59.673 | 1.00 | 43.32 |
| | 1477 | CD11 | ILE | 173 | 121.040 | 9.829 | 62.553 | 1.00 | 58.82 |
| 30 | 1478 | H | ILE | 173 | 121.833 | 11.884 | 58.002 | 1.00 | 25.00 |
| | 1479 | N | HIS | 174 | 124.848 | 10.790 | 59.020 | 1.00 | 27.02 |
| | 1480 | CA | HIS | 174 | 126.220 | 10.309 | 59.100 | 1.00 | 30.73 |
| | 1481 | C | HIS | 174 | 127.251 | 11.412 | 58.870 | 1.00 | 30.72 |
| | 1482 | O | HIS | 174 | 128.261 | 11.477 | 59.574 | 1.00 | 32.05 |
| 35 | 1483 | CB | HIS | 174 | 126.431 | 9.118 | 58.166 | 1.00 | 32.72 |
| | 1484 | CG | HIS | 174 | 125.701 | 7.884 | 58.603 | 1.00 | 42.58 |
| | 1485 | ND1 | HIS | 174 | 125.738 | 7.418 | 59.902 | 1.00 | 43.81 |
| | 1486 | CD2 | HIS | 174 | 124.891 | 7.036 | 57.925 | 1.00 | 39.61 |
| | 1487 | CE1 | HIS | 174 | 124.981 | 6.339 | 60.005 | 1.00 | 38.39 |
| 40 | 1488 | NE2 | HIS | 174 | 124.457 | 6.086 | 58.820 | 1.00 | 38.65 |
| | 1489 | H | HIS | 174 | 124.304 | 10.608 | 58.221 | 1.00 | 25.00 |
| | 1490 | HD1 | HIS | 174 | 126.233 | 7.787 | 60.656 | 1.00 | 25.00 |
| | 1491 | HE2 | HIS | 174 | 123.858 | 5.338 | 58.611 | 1.00 | 25.00 |
| | 1492 | N | LEU | 175 | 126.970 | 12.310 | 57.931 | 1.00 | 30.47 |
| 45 | 1493 | CA | LEU | 175 | 127.874 | 13.420 | 57.655 | 1.00 | 24.51 |
| | 1494 | C | LEU | 175 | 127.926 | 14.333 | 58.880 | 1.00 | 23.90 |
| | 1495 | O | LEU | 175 | 128.999 | 14.803 | 59.267 | 1.00 | 27.49 |
| | 1496 | CB | LEU | 175 | 127.429 | 14.193 | 56.408 | 1.00 | 18.74 |
| | 1497 | CG | LEU | 175 | 127.687 | 13.517 | 55.054 | 1.00 | 19.75 |
| 50 | 1498 | CD1 | LEU | 175 | 127.007 | 14.295 | 53.935 | 1.00 | 19.14 |
| | 1499 | CD2 | LEU | 175 | 129.187 | 13.404 | 54.789 | 1.00 | 13.66 |
| | 1500 | H | LEU | 175 | 126.143 | 12.235 | 57.409 | 1.00 | 25.00 |

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|----|------|-----|-----|-----|----------|--------|--------|------|-------|
| | 1501 | N | GLU | 176 | 126.781 | 14.535 | 59.524 | 1.00 | 23.45 |
| | 1502 | CA | GLU | 176 | 126.7221 | 15.374 | 60.717 | 1.00 | 29.31 |
| | 1503 | C | GLU | 176 | 127.596 | 14.788 | 61.814 | 1.00 | 29.58 |
| | 1504 | O | GLU | 176 | 128.222 | 15.519 | 62.580 | 1.00 | 30.33 |
| 5 | 1505 | CB | GLU | 176 | 125.292 | 15.477 | 61.247 | 1.00 | 28.86 |
| | 1506 | CG | GLU | 176 | 124.338 | 16.265 | 60.381 | 1.00 | 41.02 |
| | 1507 | CD | GLU | 176 | 122.976 | 16.431 | 61.032 | 1.00 | 50.96 |
| | 1508 | OE1 | GLU | 176 | 122.409 | 15.422 | 61.511 | 1.00 | 58.24 |
| | 1509 | OE2 | GLU | 176 | 122.474 | 17.574 | 61.069 | 1.00 | 53.02 |
| 10 | 1510 | H | GLU | 176 | 125.956 | 14.127 | 59.182 | 1.00 | 25.00 |
| | 1511 | N | SER | 177 | 127.615 | 13.461 | 61.890 | 1.00 | 31.99 |
| | 1512 | CA | SER | 177 | 128.394 | 12.746 | 62.894 | 1.00 | 33.70 |
| | 1513 | C | SER | 177 | 129.905 | 12.777 | 62.620 | 1.00 | 29.73 |
| | 1514 | O | SER | 177 | 130.710 | 12.952 | 63.541 | 1.00 | 31.31 |
| 15 | 1515 | CB | SER | 177 | 127.896 | 11.299 | 62.986 | 1.00 | 33.08 |
| | 1516 | OG | SER | 177 | 128.446 | 10.626 | 64.103 | 1.00 | 42.66 |
| | 1517 | H | SER | 177 | 127.077 | 12.944 | 61.259 | 1.00 | 25.00 |
| | 1518 | HG | SER | 177 | 128.220 | 11.094 | 64.907 | 1.00 | 25.00 |
| | 1519 | N | ALA | 178 | 130.283 | 12.652 | 61.352 | 1.00 | 26.67 |
| 20 | 1520 | CA | ALA | 178 | 131.692 | 12.641 | 60.970 | 1.00 | 25.61 |
| | 1521 | C | ALA | 178 | 132.351 | 14.013 | 60.858 | 1.00 | 28.58 |
| | 1522 | O | ALA | 178 | 133.540 | 14.162 | 61.153 | 1.00 | 23.60 |
| | 1523 | CB | ALA | 178 | 131.862 | 11.884 | 59.665 | 1.00 | 22.60 |
| | 1524 | H | ALA | 178 | 129.599 | 12.566 | 60.656 | 1.00 | 25.00 |
| 25 | 1525 | N | ALA | 179 | 131.568 | 15.018 | 60.475 | 1.00 | 25.11 |
| | 1526 | CA | ALA | 179 | 132.068 | 16.376 | 60.268 | 1.00 | 25.17 |
| | 1527 | C | ALA | 179 | 133.071 | 16.983 | 61.254 | 1.00 | 25.37 |
| | 1528 | O | ALA | 179 | 134.141 | 17.430 | 60.844 | 1.00 | 25.58 |
| | 1529 | CB | ALA | 179 | 130.903 | 17.340 | 60.044 | 1.00 | 21.50 |
| 30 | 1530 | H | ALA | 179 | 130.617 | 14.840 | 60.325 | 1.00 | 25.00 |
| | 1531 | N | PRO | 180 | 132.771 | 16.963 | 62.564 | 1.00 | 27.61 |
| | 1532 | CA | PRO | 180 | 133.680 | 17.541 | 63.565 | 1.00 | 28.57 |
| | 1533 | C | PRO | 180 | 135.132 | 17.058 | 63.584 | 1.00 | 30.64 |
| | 1534 | O | PRO | 180 | 135.994 | 17.724 | 64.155 | 1.00 | 37.22 |
| 35 | 1535 | CB | PRO | 180 | 132.988 | 17.206 | 64.889 | 1.00 | 25.80 |
| | 1536 | CG | PRO | 180 | 131.540 | 17.118 | 64.518 | 1.00 | 31.06 |
| | 1537 | CD | PRO | 180 | 131.597 | 16.360 | 63.221 | 1.00 | 30.35 |
| | 1538 | N | HIS | 181 | 135.414 | 15.910 | 62.980 | 1.00 | 28.35 |
| | 1539 | CA | HIS | 181 | 136.772 | 15.377 | 63.013 | 1.00 | 27.57 |
| 40 | 1540 | C | HIS | 181 | 137.470 | 15.237 | 61.672 | 1.00 | 26.99 |
| | 1541 | O | HIS | 181 | 138.529 | 14.611 | 61.584 | 1.00 | 29.22 |
| | 1542 | CB | HIS | 181 | 136.764 | 14.035 | 63.740 | 1.00 | 30.76 |
| | 1543 | CG | HIS | 181 | 136.153 | 14.103 | 65.104 | 1.00 | 32.51 |
| | 1544 | ND1 | HIS | 181 | 134.893 | 13.619 | 65.379 | 1.00 | 34.64 |
| 45 | 1545 | CD2 | HIS | 181 | 136.607 | 14.652 | 66.257 | 1.00 | 34.04 |
| | 1546 | CE1 | HIS | 181 | 134.593 | 13.870 | 66.641 | 1.00 | 35.16 |
| | 1547 | NE2 | HIS | 181 | 135.615 | 14.495 | 67.196 | 1.00 | 38.60 |
| | 1548 | H | HIS | 181 | 134.717 | 15.429 | 62.478 | 1.00 | 25.00 |
| | 1549 | HD1 | HIS | 181 | 134.298 | 13.158 | 64.739 | 1.00 | 25.00 |
| 50 | 1550 | HE2 | HIS | 181 | 135.666 | 14.802 | 68.128 | 1.00 | 25.00 |
| | 1551 | N | LEU | 182 | 136.890 | 15.827 | 60.635 | 1.00 | 22.56 |
| | 1552 | CA | LEU | 182 | 137.468 | 15.750 | 59.303 | 1.00 | 22.65 |

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|----|------|-----|------|-----|---------|--------|--------|------|-------|
| | 1553 | C | LEU | 182 | 138.532 | 16.821 | 59.103 | 1.00 | 24.98 |
| | 1554 | O | LEU | 182 | 138.494 | 17.878 | 59.741 | 1.00 | 22.99 |
| | 1555 | CB | LEU | 182 | 136.372 | 15.900 | 58.243 | 1.00 | 25.05 |
| | 1556 | CG | LEU | 182 | 135.271 | 14.835 | 58.205 | 1.00 | 23.65 |
| 5 | 1557 | CD1 | LEU | 182 | 134.178 | 15.274 | 57.249 | 1.00 | 17.28 |
| | 1558 | CD2 | LEU | 182 | 135.849 | 13.483 | 57.786 | 1.00 | 20.03 |
| | 1559 | H | LEU | 182 | 136.072 | 16.351 | 60.762 | 1.00 | 25.00 |
| | 1560 | N | LYS | 183 | 139.494 | 16.528 | 58.236 | 1.00 | 22.16 |
| | 1561 | CA | LYS | 183 | 140.556 | 17.469 | 57.926 | 1.00 | 25.90 |
| 10 | 1562 | C | LYS | 183 | 139.982 | 18.573 | 57.045 | 1.00 | 30.39 |
| | 1563 | O | LYS | 183 | 138.898 | 18.429 | 56.468 | 1.00 | 31.71 |
| | 1564 | CB | LYS | 183 | 141.696 | 16.767 | 57.183 | 1.00 | 27.62 |
| | 1565 | CG | LYS | 183 | 141.274 | 16.122 | 55.871 | 1.00 | 37.10 |
| | 1566 | CD | LYS | 183 | 142.437 | 15.441 | 55.169 | 1.00 | 45.13 |
| 15 | 1567 | CE | LYS | 183 | 141.974 | 14.764 | 53.885 | 1.00 | 50.33 |
| | 1568 | NZ | LYS | 183 | 143.088 | 14.040 | 53.210 | 1.00 | 57.79 |
| | 1569 | H | LYS | 183 | 139.473 | 15.658 | 57.786 | 1.00 | 25.00 |
| | 1570 | 1HZ | LYS | 183 | 143.846 | 14.713 | 52.975 | 1.00 | 25.00 |
| | 1571 | 2HZ | LYS | 183 | 143.463 | 13.311 | 53.852 | 1.00 | 25.00 |
| 20 | 1572 | 3HZ | LYS | 183 | 142.736 | 13.592 | 52.341 | 1.00 | 25.00 |
| | 1573 | N | SER | 184 | 140.714 | 19.674 | 56.944 | 1.00 | 27.77 |
| | 1574 | CA | SER | 184 | 140.304 | 20.802 | 56.122 | 1.00 | 28.80 |
| | 1575 | C | SER | 184 | 140.970 | 20.675 | 54.752 | 1.00 | 27.61 |
| | 1576 | O | SER | 184 | 142.084 | 20.158 | 54.645 | 1.00 | 26.37 |
| 25 | 1577 | CB | SER | 184 | 140.702 | 22.109 | 56.805 | 1.00 | 28.03 |
| | 1578 | OG | SEER | 184 | 140.003 | 22.254 | 58.031 | 1.00 | 32.93 |
| | 1579 | H | SER | 184 | 141.565 | 19.725 | 57.420 | 1.00 | 25.00 |
| | 1580 | HG | SER | 184 | 140.193 | 21.517 | 58.620 | 1.00 | 25.00 |
| | 1581 | N | PRO | 185 | 140.312 | 21.171 | 53.689 | 1.00 | 26.21 |
| 30 | 1582 | CA | PRO | 185 | 139.003 | 21.834 | 53.680 | 1.00 | 23.45 |
| | 1583 | C | PRO | 185 | 137.767 | 20.926 | 53.597 | 1.00 | 24.54 |
| | 1584 | O | PRO | 185 | 136.636 | 21.425 | 53.589 | 1.00 | 23.22 |
| | 1585 | CB | PRO | 185 | 139.109 | 22.737 | 52.458 | 1.00 | 21.98 |
| | 1586 | CG | PRO | 185 | 139.858 | 21.876 | 51.503 | 1.00 | 21.03 |
| 35 | 1587 | CD | PRO | 185 | 140.949 | 21.263 | 52.361 | 1.00 | 21.80 |
| | 1588 | N | LEU | 186 | 137.969 | 19.608 | 53.570 | 1.00 | 21.43 |
| | 1589 | CA | LEU | 186 | 136.852 | 18.666 | 53.483 | 1.00 | 21.42 |
| | 1590 | C | LEU | 186 | 135.780 | 18.964 | 54.522 | 1.00 | 22.24 |
| | 1591 | O | LEU | 186 | 134.586 | 18.987 | 54.210 | 1.00 | 20.84 |
| 40 | 1592 | CB | LEU | 186 | 137.331 | 17.220 | 53.654 | 1.00 | 23.63 |
| | 1593 | CG | LEU | 186 | 136.217 | 16.160 | 53.646 | 1.00 | 21.09 |
| | 1594 | CD1 | LEU | 186 | 135.491 | 16.145 | 52.292 | 1.00 | 20.03 |
| | 1595 | CD2 | LEU | 186 | 136.800 | 14.800 | 53.943 | 1.00 | 21.57 |
| | 1596 | H | LEU | 186 | 138.882 | 19.259 | 53.605 | 1.00 | 25.00 |
| 45 | 1597 | N | ARG | 187 | 136.221 | 19.208 | 55.751 | 1.00 | 16.73 |
| | 1598 | CA | ARG | 187 | 135.326 | 19.515 | 56.859 | 1.00 | 22.57 |
| | 1599 | C | ARG | 187 | 134.427 | 20.723 | 56.564 | 1.00 | 27.49 |
| | 1600 | O | ARG | 187 | 133.225 | 20.693 | 56.848 | 1.00 | 26.35 |
| | 1601 | CB | ARG | 187 | 136.146 | 19.777 | 58.117 | 1.00 | 17.71 |
| 50 | 1602 | CG | ARG | 187 | 135.325 | 20.087 | 59.343 | 1.00 | 21.93 |
| | 1603 | CD | ARG | 187 | 136.235 | 20.478 | 60.483 | 1.00 | 31.75 |
| | 1604 | NE | ARG | 187 | 135.507 | 20.685 | 61.727 | 1.00 | 46.15 |

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|----|-------|------|-----|-----|---------|--------|--------|------|-------|
| | 1605 | CZ | ARG | 187 | 136.087 | 20.961 | 62.891 | 1.00 | 58.70 |
| | 1606 | NH1 | ARG | 187 | 137.412 | 21.066 | 62.970 | 1.00 | 57.84 |
| | 1607 | NH2 | ARG | 187 | 135.344 | 21.111 | 63.982 | 1.00 | 58.69 |
| 5 | 1608 | H | ARG | 187 | 137.182 | 19.161 | 55.923 | 1.00 | 25.00 |
| | 1609 | HE | ARG | 187 | 134.530 | 20.613 | 61.708 | 1.00 | 25.00 |
| | 1610 | 1HH1 | ARG | 187 | 137.977 | 20.941 | 62.156 | 1.00 | 25.00 |
| | 1611 | 2HH1 | ARG | 187 | 137.843 | 21.275 | 63.848 | 1.00 | 25.00 |
| | 1612 | 1HH2 | ARG | 187 | 134.351 | 21.012 | 63.926 | 1.00 | 25.00 |
| 10 | 1613 | 2HH2 | ARG | 187 | 135.779 | 21.316 | 64.858 | 1.00 | 25.00 |
| | 1614 | N | GLU | 188 | 135.010 | 21.782 | 56.001 | 1.00 | 28.09 |
| | 1615 | CA | GLU | 188 | 134.255 | 22.993 | 55.667 | 1.00 | 26.62 |
| | 16116 | C | GLU | 188 | 133.293 | 22.726 | 54.516 | 1.00 | 22.97 |
| | 1617 | O | GLU | 188 | 132.203 | 23.296 | 54.462 | 1.00 | 21.14 |
| | 1618 | CB | GLU | 188 | 135.192 | 24.153 | 55.305 | 1.00 | 24.01 |
| 15 | 1619 | CG | GLU | 188 | 135.934 | 24.768 | 56.482 | 1.00 | 32.71 |
| | 1620 | CD | GLU | 188 | 137.045 | 23.878 | 57.014 | 1.00 | 42.50 |
| | 1621 | OE1 | GLU | 188 | 138.030 | 23.657 | 56.279 | 1.00 | 43.53 |
| | 1622 | OE2 | GLU | 188 | 136.936 | 23.403 | 58.165 | 1.00 | 47.38 |
| | 1623 | H | GLU | 188 | 135.965 | 21.747 | 55.798 | 1.00 | 25.00 |
| 20 | 1624 | N | GLN | 189 | 133.702 | 21.853 | 53.601 | 1.00 | 19.36 |
| | 1625 | CA | GLN | 189 | 132.872 | 21.496 | 52.460 | 1.00 | 20.62 |
| | 1626 | C | GLN | 189 | 131.636 | 20.728 | 52.927 | 1.00 | 22.47 |
| | 1627 | O | GLN | 189 | 130.522 | 21.010 | 52.483 | 1.00 | 25.58 |
| | 1628 | CB | GLN | 189 | 133.672 | 20.662 | 51.461 | 1.00 | 17.31 |
| 25 | 1629 | CG | GLN | 189 | 132.915 | 20.359 | 50.187 | 1.00 | 24.12 |
| | 1630 | CD | GLN | 189 | 133.796 | 19.780 | 49.104 | 1.00 | 25.67 |
| | 1631 | OE1 | GLN | 189 | 133.691 | 20.162 | 47.939 | 1.00 | 28.92 |
| | 1632 | NE2 | GLN | 189 | 134.666 | 18.850 | 49.477 | 1.00 | 28.68 |
| | 1633 | H | GLN | 189 | 134.590 | 21.445 | 53.695 | 1.00 | 25.00 |
| 30 | 1634 | 1HE2 | GLN | 189 | 135.235 | 18.480 | 48.773 | 1.00 | 25.00 |
| | 1635 | 2HE2 | GLN | 189 | 134.704 | 18.576 | 50.413 | 1.00 | 25.00 |
| | 1636 | N | VAL | 190 | 131.833 | 19.783 | 53.846 | 1.00 | 22.03 |
| | 1637 | CA | VAL | 190 | 130.734 | 18.983 | 54.388 | 1.00 | 22.50 |
| | 1638 | C | VAL | 190 | 129.778 | 19.864 | 55.198 | 1.00 | 22.00 |
| 35 | 1639 | O | VAL | 190 | 128.565 | 19.846 | 54.977 | 1.00 | 26.49 |
| | 1640 | CB | VAL | 190 | 131.255 | 17.808 | 55.274 | 1.00 | 18.21 |
| | 1641 | CG1 | VAL | 190 | 130.093 | 17.093 | 55.947 | 1.00 | 19.13 |
| | 1642 | CG2 | VAL | 190 | 132.037 | 16.815 | 54.422 | 1.00 | 13.74 |
| | 1643 | H | VAL | 190 | 132.742 | 19.618 | 54.168 | 1.00 | 25.00 |
| 40 | 1644 | N | THR | 191 | 130.335 | 20.638 | 56.124 | 1.00 | 20.35 |
| | 1645 | CA | THR | 191 | 129.555 | 21.541 | 56.967 | 1.00 | 23.43 |
| | 1646 | C | THR | 191 | 128.733 | 22.504 | 56.116 | 1.00 | 23.79 |
| | 1647 | O | THR | 191 | 127.564 | 22.772 | 56.410 | 1.00 | 27.12 |
| | 1648 | CB | THR | 191 | 130.478 | 22.350 | 57.903 | 1.00 | 29.00 |
| 45 | 1649 | OG1 | THR | 191 | 131.124 | 21.454 | 58.814 | 1.00 | 35.12 |
| | 1650 | CG2 | THR | 191 | 129.688 | 23.385 | 58.691 | 1.00 | 32.22 |
| | 1651 | H | THR | 191 | 131.304 | 20.599 | 56.257 | 1.00 | 25.00 |
| | 1652 | HG1 | THR | 191 | 131.661 | 20.824 | 58.321 | 1.00 | 25.00 |
| | 1653 | N | HIS | 192 | 129.345 | 23.015 | 55.054 | 1.00 | 22.27 |
| 50 | 1654 | CA | HIS | 192 | 128.658 | 23.935 | 54.168 | 1.00 | 24.21 |
| | 1655 | C | HIS | 192 | 127.530 | 23.226 | 53.417 | 1.00 | 24.78 |
| | 1656 | O | HIS | 192 | 126.421 | 23.756 | 53.326 | 1.00 | 20.41 |

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|----|------|------|-----|-----|---------|--------|---------|------|-------|
| | 1657 | CB | HIS | 192 | 129.632 | 24.564 | 53.173 | 1.00 | 17.98 |
| | 1658 | CG | HIS | 192 | 128.965 | 25.446 | 52.169 | 1.00 | 21.55 |
| | 1659 | ND1 | HIS | 192 | 128.506 | 26.707 | 52.480 | 1.00 | 21.86 |
| 5 | 1660 | CD2 | HIS | 192 | 128.637 | 25.234 | 50.872 | 1.00 | 20.40 |
| | 1661 | CE1 | HIS | 192 | 127.919 | 27.234 | 51.420 | 1.00 | 20.03 |
| | 1662 | NE2 | HIS | 192 | 127.985 | 26.360 | 50.432 | 1.00 | 20.23 |
| | 1663 | H | HIS | 192 | 130.278 | 22.766 | 54.870 | 1.00 | 25.00 |
| | 1664 | HD1 | HIS | 192 | 128.594 | 27.143 | 53.355 | 1.00 | 25.00 |
| | 1665 | HE2 | HIS | 192 | 127.614 | 26.486 | 49.551 | 1.00 | 25.00 |
| 10 | 1666 | N | ALA | 193 | 127.826 | 22.038 | 52.8888 | 1.00 | 22.45 |
| | 1667 | CA | ALA | 193 | 126.854 | 21.242 | 52.139 | 1.00 | 20.56 |
| | 1668 | C | ALA | 193 | 125.601 | 20.963 | 52.964 | 1.00 | 22.26 |
| | 1669 | O | ALA | 193 | 124.485 | 21.072 | 52.459 | 1.00 | 21.49 |
| | 1670 | CB | ALA | 193 | 127.483 | 19.938 | 51.679 | 1.00 | 18.73 |
| 15 | 1671 | H | ALA | 193 | 128.729 | 21.672 | 53.002 | 1.00 | 25.00 |
| | 1672 | N | LEU | 194 | 125.791 | 20.623 | 54.236 | 1.00 | 23.86 |
| | 1673 | CA | LEU | 194 | 124.678 | 20.344 | 55.136 | 1.00 | 25.16 |
| | 1674 | C | LEU | 194 | 123.757 | 21.551 | 55.298 | 1.00 | 26.76 |
| | 1675 | O | LEU | 194 | 122.573 | 21.391 | 55.579 | 1.00 | 28.61 |
| 20 | 1676 | CB | LEU | 194 | 125.194 | 19.902 | 56.509 | 1.00 | 23.10 |
| | 1677 | CG | LEU | 194 | 125.924 | 18.556 | 56.579 | 1.00 | 26.60 |
| | 1678 | CD1 | LEU | 194 | 126.426 | 18.319 | 57.992 | 1.00 | 20.06 |
| | 1679 | CD2 | LEU | 194 | 124.998 | 17.433 | 56.149 | 1.00 | 18.24 |
| | 1680 | H | LEU | 194 | 126.710 | 20.552 | 54.574 | 1.00 | 25.00 |
| 25 | 1681 | N | GLU | 195 | 124.309 | 22.754 | 55.149 | 1.00 | 33.01 |
| | 1682 | CA | GLU | 195 | 123.529 | 23.987 | 55.277 | 1.00 | 34.61 |
| | 1683 | C | GLU | 195 | 123.005 | 24.448 | 53.923 | 1.00 | 26.09 |
| | 1684 | O | GLU | 195 | 121.952 | 25.074 | 53.834 | 1.00 | 29.66 |
| | 1685 | CB | GLU | 195 | 124.385 | 25.102 | 55.884 | 1.00 | 38.35 |
| 30 | 1686 | CG | GLU | 195 | 124.885 | 24.816 | 57.288 | 1.00 | 59.66 |
| | 1687 | CD | GLU | 195 | 125.945 | 25.803 | 57.751 | 1.00 | 72.22 |
| | 1688 | OE1 | GLU | 195 | 126.800 | 26.203 | 56.927 | 1.00 | 75.42 |
| | 1689 | OE2 | GLU | 195 | 125.931 | 26.169 | 58.947 | 1.00 | 82.70 |
| | 1690 | H | GLU | 195 | 125.263 | 22.814 | 54.944 | 1.00 | 25.00 |
| 35 | 1691 | N | GLN | 196 | 123.747 | 24.130 | 52.871 | 1.00 | 22.78 |
| | 1692 | CA | GLN | 196 | 123.376 | 24.529 | 51.527 | 1.00 | 20.33 |
| | 1693 | C | GLN | 196 | 123.891 | 23.520 | 50.515 | 1.00 | 19.79 |
| | 1694 | O | GLN | 196 | 125.094 | 23.463 | 50.258 | 1.00 | 24.78 |
| | 1695 | CB | GLN | 196 | 123.980 | 25.903 | 51.219 | 1.00 | 20.38 |
| 40 | 1696 | CG | GLN | 196 | 123.727 | 26.397 | 49.807 | 1.00 | 24.47 |
| | 1697 | CD | GLN | 196 | 122.253 | 26.591 | 49.524 | 1.00 | 28.74 |
| | 1698 | OE1 | GLN | 196 | 121.622 | 27.490 | 50.074 | 1.00 | 32.30 |
| | 1699 | NE2 | GLN | 196 | 121.694 | 25.744 | 48.667 | 1.00 | 21.06 |
| | 1700 | H | GLN | 196 | 124.554 | 23.592 | 52.995 | 1.00 | 25.00 |
| 45 | 1701 | 1HE2 | GLN | 196 | 120.741 | 25.876 | 48.480 | 1.00 | 25.00 |
| | 1702 | 2HE2 | GLN | 196 | 122.247 | 25.045 | 48.258 | 1.00 | 25.00 |
| | 1703 | N | CYS | 197 | 122.992 | 22.727 | 49.942 | 1.00 | 19.52 |
| | 1704 | CA | CYS | 197 | 123.399 | 21.749 | 48.944 | 1.00 | 17.94 |
| | 1705 | C | CYS | 197 | 123.782 | 22.497 | 47.669 | 1.00 | 18.82 |
| 50 | 1706 | O | CYS | 197 | 123.316 | 23.614 | 47.428 | 1.00 | 19.62 |
| | 1707 | CB | CYS | 197 | 122.278 | 20.743 | 48.669 | 1.00 | 21.42 |
| | 1708 | SG | CYS | 197 | 120.832 | 21.394 | 47.800 | 1.00 | 42.82 |

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|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 1709 | H | CYS | 197 | 122.056 | 22.808 | 50.202 | 1.00 | 25.00 |
| | 1710 | N | LEU | 198 | 124.626 | 21.878 | 46.856 | 1.00 | 19.01 |
| | 1711 | CA | LEU | 198 | 125.094 | 22.489 | 45.620 | 1.00 | 20.23 |
| | 1712 | C | LEU | 198 | 123.986 | 22.760 | 44.610 | 1.00 | 23.16 |
| 5 | 1713 | O | LEU | 198 | 123.868 | 23.867 | 44.096 | 1.00 | 26.68 |
| | 1714 | CB | LEU | 198 | 126.174 | 21.608 | 44.981 | 1.00 | 13.53 |
| | 1715 | CG | LEU | 198 | 126.762 | 22.058 | 43.640 | 1.00 | 20.37 |
| | 1716 | CD1 | LEU | 198 | 127.388 | 23.440 | 43.773 | 1.00 | 19.35 |
| | 1717 | CD2 | LEU | 198 | 127.789 | 21.044 | 43.158 | 1.00 | 18.28 |
| 10 | 1718 | H | LEU | 198 | 124.968 | 21.004 | 47.109 | 1.00 | 25.00 |
| | 1719 | N | HIS | 199 | 123.160 | 21.752 | 44.354 | 1.00 | 24.27 |
| | 1720 | CA | HIS | 199 | 122.079 | 21.859 | 43.379 | 1.00 | 22.48 |
| | 1721 | C | HIS | 199 | 121.089 | 23.001 | 43.608 | 1.00 | 19.15 |
| | 1722 | O | HIS | 199 | 120.586 | 23.582 | 42.653 | 1.00 | 19.66 |
| 15 | 1723 | CB | HIS | 199 | 121.327 | 20.523 | 43.277 | 1.00 | 22.51 |
| | 1724 | CG | HIS | 199 | 120.225 | 20.519 | 42.261 | 1.00 | 16.72 |
| | 1725 | ND1 | HIS | 199 | 120.452 | 20.697 | 40.911 | 1.00 | 19.56 |
| | 1726 | CD2 | HIS | 199 | 118.885 | 20.360 | 42.396 | 1.00 | 15.14 |
| | 1727 | CE1 | HIS | 199 | 119.303 | 20.648 | 40.261 | 1.00 | 15.68 |
| 20 | 1728 | NE2 | HIS | 199 | 118.338 | 20.444 | 41.138 | 1.00 | 19.96 |
| | 1729 | H | HIS | 199 | 123.297 | 20.912 | 44.822 | 1.00 | 25.00 |
| | 1730 | HD1 | HIS | 199 | 121.340 | 20.834 | 40.498 | 1.00 | 25.00 |
| | 1731 | HE2 | HIS | 199 | 117.376 | 20.343 | 40.929 | 1.00 | 25.00 |
| | 1732 | N | LYS | 200 | 120.811 | 23.323 | 44.864 | 1.00 | 18.06 |
| 25 | 1733 | CA | LYS | 200 | 119.853 | 24.377 | 45.170 | 1.00 | 19.34 |
| | 1734 | C | LYS | 200 | 120.463 | 25.726 | 45.548 | 1.00 | 21.28 |
| | 1735 | O | LYS | 200 | 119.755 | 26.617 | 46.012 | 1.00 | 20.62 |
| | 1736 | CB | LYS | 200 | 118.898 | 23.893 | 46.264 | 1.00 | 17.06 |
| | 1737 | CG | LYS | 200 | 118.144 | 22.630 | 45.875 | 1.00 | 17.06 |
| 30 | 1738 | CD | LYS | 200 | 117.287 | 22.086 | 47.005 | 1.00 | 18.82 |
| | 1739 | CE | LYS | 200 | 116.597 | 20.804 | 46.559 | 1.00 | 16.83 |
| | 1740 | NZ | LYS | 200 | 115.820 | 20.155 | 47.645 | 1.00 | 19.41 |
| | 1741 | H | LYS | 200 | 121.264 | 22.869 | 45.599 | 1.00 | 25.00 |
| | 1742 | 1HZ | LYS | 200 | 116.454 | 19.923 | 48.436 | 1.00 | 25.00 |
| 35 | 1743 | 2HZ | LYS | 200 | 115.081 | 20.807 | 47.978 | 1.00 | 25.00 |
| | 1744 | 3HZ | LYS | 200 | 115.377 | 19.285 | 47.288 | 1.00 | 25.00 |
| | 1745 | N | GLY | 201 | 121.768 | 25.881 | 45.343 | 1.00 | 23.54 |
| | 1746 | CA | GLY | 201 | 122.424 | 27.136 | 45.675 | 1.00 | 19.60 |
| | 1747 | C | GLY | 201 | 122.583 | 28.062 | 44.482 | 1.00 | 19.35 |
| 40 | 1748 | O | GLY | 201 | 122.569 | 27.613 | 43.338 | 1.00 | 21.61 |
| | 1749 | H | GLY | 201 | 122.299 | 25.166 | 44.933 | 1.00 | 25.00 |
| | 1750 | N | VAL | 202 | 122.685 | 29.363 | 44.734 | 1.00 | 17.34 |
| | 1751 | CA | VAL | 202 | 122.871 | 30.327 | 43.653 | 1.00 | 17.16 |
| | 1752 | C | VAL | 202 | 124.281 | 30.084 | 43.108 | 1.00 | 20.63 |
| 45 | 1753 | O | VAL | 202 | 125.248 | 30.059 | 43.874 | 1.00 | 22.87 |
| | 1754 | CB | VAL | 202 | 122.722 | 31.778 | 44.168 | 1.00 | 17.85 |
| | 1755 | CG1 | VAL | 202 | 123.062 | 32.782 | 43.071 | 1.00 | 19.32 |
| | 1756 | CG2 | VAL | 202 | 121.301 | 32.003 | 44.645 | 1.00 | 15.75 |
| | 1757 | H | VAL | 202 | 122.625 | 29.676 | 45.655 | 1.00 | 25.00 |
| 50 | 1758 | N | PRO | 203 | 124.414 | 29.905 | 41.780 | 1.00 | 18.06 |
| | 1759 | CA | PRO | 203 | 125.705 | 29.652 | 41.128 | 1.00 | 19.86 |
| | 1760 | C | PRO | 203 | 126.889 | 30.506 | 41.588 | 1.00 | 23.15 |

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|----|------|------|-----|------|---------|---------|--------|------|-------|
| | 1761 | O | PRO | 203 | 127.827 | 29.974 | 42.172 | 1.00 | 27.00 |
| | 1762 | CB | PRO | 203 | 125.378 | 29.840 | 39.650 | 1.00 | 21.47 |
| | 1763 | CG | PRO | 203 | 123.982 | 29.300 | 39.574 | 1.00 | 19.55 |
| | 1764 | CD | PRO | 203 | 123.332 | 29.952 | 40.780 | 1.00 | 17.62 |
| 5 | 1765 | N | ARG | 204 | 126.844 | 31.817 | 41.365 | 1.00 | 21.91 |
| | 1766 | CA | ARG | 204 | 127.949 | 32.683 | 41.781 | 1.00 | 20.91 |
| | 1767 | C | ARG | 204 | 128.283 | 32.568 | 43.265 | 1.00 | 20.45 |
| | 1768 | O | ARG | 204 | 129.455 | 32.598 | 43.638 | 1.00 | 25.04 |
| | 1769 | CB | ARG | 204 | 127.681 | 34.149 | 41.426 | 1.00 | 22.61 |
| 10 | 1770 | CG | ARG | 204 | 127.940 | 34.519 | 39.972 | 1.00 | 18.14 |
| | 1771 | CD | ARG | 204 | 129.420 | 34.487 | 39.618 | 1.00 | 21.89 |
| | 1772 | NE | ARG | 204 | 129.852 | 33.202 | 39.074 | 1.00 | 23.42 |
| | 1773 | CZ | ARG | 204 | 130.953 | 33.027 | 38.345 | 1.00 | 28.33 |
| | 1774 | NH1 | ARG | 204 | 131.747 | 34.055 | 38.069 | 1.00 | 25.07 |
| 15 | 1775 | NH2 | ARG | 204 | 131.248 | 31.827 | 37.862 | 1.00 | 26.89 |
| | 1776 | H | ARG | 204 | 126.071 | 32.201 | 40.913 | 1.00 | 25.00 |
| | 1777 | HE | ARG | 204 | 129.297 | 32.416 | 39.258 | 1.00 | 25.00 |
| | 1778 | 1HH1 | ARG | 204 | 131.521 | 34.967 | 38.404 | 1.00 | 25.00 |
| | 1779 | 2HH1 | ARG | 204 | 132.570 | 33.921 | 37.522 | 1.00 | 25.00 |
| 20 | 1780 | 1HH2 | ARG | 2004 | 130.647 | 31.051 | 38.047 | 1.00 | 25.00 |
| | 1781 | 2HH2 | ARG | 204 | 132.077 | 31.699 | 37.316 | 1.00 | 25.00 |
| | 1782 | N | VAL | 205 | 127.264 | 32.431 | 44.108 | 1.00 | 17.32 |
| | 1783 | CA | VAL | 205 | 127.496 | 32.312 | 45.545 | 1.00 | 18.99 |
| | 1784 | C | VAL | 205 | 128.267 | 31.034 | 45.866 | 1.00 | 20.53 |
| 25 | 1785 | O | VAL | 205 | 129.220 | 31.048 | 46.647 | 1.00 | 24.18 |
| | 1786 | CB | VAL | 205 | 126.175 | 32.309 | 46.339 | 1.00 | 19.83 |
| | 1787 | CG1 | VAL | 205 | 126.442 | 32.022 | 47.811 | 1.00 | 14.97 |
| | 1788 | CG2 | VAL | 205 | 125.473 | 33.642 | 46.190 | 1.00 | 21.52 |
| | 1789 | H | VAL | 205 | 126.353 | 32.398 | 43.764 | 1.00 | 25.00 |
| 30 | 1790 | N | GLU | 206 | 127.862 | 29.933 | 45.249 | 1.00 | 22.23 |
| | 1791 | CA | GLU | 206 | 128.519 | 28.649 | 45.478 | 1.00 | 22.70 |
| | 1792 | C | GLU | 206 | 129.919 | 28.601 | 44.876 | 1.00 | 18.65 |
| | 1793 | O | GLU | 206 | 130.836 | 28.029 | 45.469 | 1.00 | 20.84 |
| | 1794 | CB | GLU | 206 | 127.648 | 27.506 | 44.957 | 1.00 | 17.73 |
| 35 | 1795 | CG | GLU | 206 | 126.317 | 27.413 | 45.683 | 1.00 | 20.17 |
| | 1796 | CD | GLU | 206 | 126.478 | 27.407 | 47.201 | 1.00 | 26.03 |
| | 1797 | OE1 | GLU | 206 | 127.190 | 26.523 | 47.721 | 1.00 | 21.64 |
| | 1798 | OE2 | GLU | 206 | 125.895 | 28.283 | 47.876 | 1.00 | 20.28 |
| | 1799 | H | GLU | 206 | 127.111 | 29.981 | 44.620 | 1.00 | 25.00 |
| 40 | 1800 | N | THR | 207 | 130.081 | 29.223 | 43.714 | 1.00 | 18.09 |
| | 1801 | CA | THR | 207 | 131.369 | 29.291 | 43.038 | 1.00 | 21.23 |
| | 1802 | C | THR | 207 | 132.373 | 30.057 | 43.909 | 1.00 | 25.71 |
| | 1803 | O | THR | 207 | 133.474 | 29.568 | 44.179 | 1.00 | 28.93 |
| | 1804 | CB | THR | 207 | 131.219 | 29.984 | 41.672 | 1.00 | 24.22 |
| 45 | 1805 | OG1 | THR | 207 | 130.529 | 29.1077 | 40.770 | 1.00 | 28.95 |
| | 1806 | CG2 | THR | 207 | 132.573 | 30.379 | 41.088 | 1.00 | 23.10 |
| | 1807 | H | THR | 207 | 129.311 | 29.644 | 43.289 | 1.00 | 25.00 |
| | 1808 | HG1 | THR | 207 | 131.030 | 28.287 | 40.685 | 1.00 | 25.00 |
| | 1809 | N | ARG | 208 | 131.973 | 31.238 | 44.374 | 1.00 | 24.65 |
| 50 | 1810 | CA | ARG | 208 | 132.825 | 32.070 | 45.221 | 1.00 | 25.56 |
| | 1811 | C | ARG | 208 | 133.292 | 31.273 | 46.432 | 1.00 | 25.87 |
| | 1812 | O | ARG | 208 | 134.472 | 31.289 | 46.780 | 1.00 | 27.73 |

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|----|------|------|-----|-----|----------|--------|--------|------|-------|
| | 1813 | CB | ARG | 208 | 132.059 | 33.314 | 45.682 | 1.00 | 25.72 |
| | 1814 | CG | ARG | 208 | 132.836 | 34.258 | 46.588 | 1.00 | 31.65 |
| | 1815 | CD | ARG | 208 | 134.062 | 34.826 | 45.892 | 1.00 | 39.53 |
| | 1816 | NE | ARG | 208 | 134.374 | 36.184 | 46.344 | 1.00 | 46.43 |
| 5 | 1817 | CZ | ARG | 208 | 135.283 | 36.488 | 47.266 | 1.00 | 47.18 |
| | 1818 | NH11 | ARG | 208 | 135.991 | 35.534 | 47.858 | 1.00 | 54.31 |
| | 1819 | NH2 | ARG | 208 | 135.492 | 37.754 | 47.592 | 1.00 | 54.01 |
| | 1820 | H | ARG | 208 | 131.077 | 31.566 | 44.139 | 1.00 | 25.00 |
| | 1821 | HE | ARG | 208 | 133.881 | 36.924 | 45.937 | 1.00 | 25.00 |
| 10 | 1822 | 1HH1 | ARG | 208 | 135.847 | 34.577 | 47.610 | 1.00 | 25.00 |
| | 1823 | 2HH1 | ARG | 208 | 136.673 | 35.775 | 48.548 | 1.00 | 25.00 |
| | 1824 | 1HH2 | ARG | 208 | 134.962 | 38.478 | 47.150 | 1.00 | 25.00 |
| | 1825 | 2HH2 | ARG | 208 | 136.172 | 37.986 | 48.287 | 1.00 | 25.00 |
| | 1826 | N | PHE | 209 | 132.364 | 30.556 | 47.056 | 1.00 | 25.17 |
| 15 | 1827 | CA | PHE | 209 | 132.688 | 29.750 | 48.224 | 1.00 | 23.72 |
| | 1828 | C | PHE | 209 | 133.677 | 28.632 | 47.908 | 1.00 | 24.69 |
| | 1829 | O | PHE | 209 | 134.656 | 28.442 | 48.626 | 1.00 | 24.23 |
| | 1830 | CB | PHE | 209 | 131.430 | 29.135 | 48.838 | 1.00 | 22.94 |
| | 1831 | CG | PHE | 209 | 131.721 | 28.195 | 49.976 | 1.00 | 22.62 |
| 20 | 1832 | CD1 | PHE | 209 | 132.019 | 28.691 | 51.242 | 1.00 | 22.83 |
| | 1833 | CD2 | PHE | 209 | 131.745 | 26.817 | 49.773 | 1.00 | 20.76 |
| | 1834 | CE1 | PHE | 209 | 132.336 | 27.824 | 52.293 | 1.00 | 22.43 |
| | 1835 | CE2 | PHE | 209 | 132.060 | 25.946 | 50.813 | 1.00 | 24.13 |
| | 1836 | CZ | PHE | 209 | 132.358 | 26.450 | 52.075 | 1.00 | 22.16 |
| 25 | 1837 | H | PHE | 209 | 131.439 | 30.580 | 46.728 | 1.00 | 25.00 |
| | 1838 | N | PHE | 210 | 133.399 | 27.872 | 46.856 | 1.00 | 24.89 |
| | 1839 | CA | PHE | 210 | 134.263 | 26.765 | 46.486 | 1.00 | 21.48 |
| | 1840 | C | PHE | 210 | 135.671 | 27.241 | 46.172 | 1.00 | 23.23 |
| | 1841 | O | PHE | 210 | 136.645 | 26.676 | 46.671 | 1.00 | 24.15 |
| 30 | 1842 | CB | PHE | 210 | 133.688 | 25.989 | 45.296 | 1.00 | 18.25 |
| | 1843 | CG | PHE | 210 | 134.4776 | 24.754 | 44.944 | 1.00 | 20.04 |
| | 1844 | CD1 | PHE | 210 | 134.506 | 23.661 | 45.811 | 1.00 | 17.95 |
| | 1845 | CD2 | PHE | 210 | 135.212 | 24.694 | 43.763 | 1.00 | 19.06 |
| | 1846 | CE1 | PHE | 210 | 135.260 | 22.525 | 45.510 | 1.00 | 17.28 |
| 35 | 1847 | CE2 | PHE | 210 | 135.972 | 23.563 | 43.450 | 1.00 | 21.18 |
| | 1848 | CZ | PHE | 210 | 135.995 | 22.476 | 44.329 | 1.00 | 18.42 |
| | 1849 | H | PHE | 210 | 132.602 | 28.062 | 46.315 | 1.00 | 25.00 |
| | 1850 | N | ILE | 211 | 135.781 | 28.290 | 45.368 | 1.00 | 26.53 |
| | 1851 | CA | ILE | 211 | 137.086 | 28.818 | 44.997 | 1.00 | 27.06 |
| 40 | 1852 | C | ILE | 211 | 137.917 | 29.248 | 46.205 | 1.00 | 27.01 |
| | 1853 | O | ILE | 211 | 138.953 | 28.652 | 46.490 | 1.00 | 25.02 |
| | 1854 | CB | ILE | 211 | 136.967 | 30.015 | 44.023 | 1.00 | 23.08 |
| | 1855 | CG1 | ILE | 211 | 136.317 | 29.574 | 42.713 | 1.00 | 22.07 |
| | 1856 | CG2 | ILE | 211 | 138.344 | 30.603 | 43.737 | 1.00 | 18.73 |
| 45 | 1857 | CD1 | ILE | 211 | 136.163 | 30.700 | 41.701 | 1.00 | 22.59 |
| | 1858 | H | ILE | 211 | 134.968 | 28.712 | 45.022 | 1.00 | 25.00 |
| | 1859 | N | SER | 212 | 137.430 | 30.233 | 46.949 | 1.00 | 26.45 |
| | 1860 | CA | SER | 212 | 138.174 | 30.758 | 48.087 | 1.00 | 29.47 |
| | 1861 | C | SER | 212 | 138.263 | 29.914 | 49.355 | 1.00 | 29.82 |
| 50 | 1862 | O | SER | 212 | 139.317 | 29.873 | 49.993 | 1.00 | 31.08 |
| | 1863 | CB | SER | 212 | 137.691 | 32.173 | 48.425 | 1.00 | 28.90 |
| | 1864 | OG | SER | 212 | 136.311 | 32.186 | 48.742 | 1.00 | 48.04 |

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|----|------|-----|-----|-----|---------|--------|---------|------|-------|
| | 1865 | H | SER | 212 | 136.550 | 30.622 | 46.740 | 1.00 | 25.00 |
| | 1866 | HG | SER | 212 | 136.156 | 31.647 | 49.517 | 1.00 | 25.00 |
| | 1867 | N | SER | 213 | 137.175 | 29.249 | 49.728 | 1.00 | 25.54 |
| | 1868 | CA | SER | 213 | 137.173 | 28.447 | 50.949 | 1.00 | 25.42 |
| 5 | 1869 | C | SER | 213 | 137.555 | 26.969 | 50.823 | 1.00 | 23.90 |
| | 1870 | O | SER | 213 | 138.019 | 26.371 | 51.794 | 1.00 | 29.58 |
| | 1871 | CB | SER | 213 | 135.820 | 28.566 | 51.662 | 1.00 | 19.77 |
| | 1872 | OG | SER | 213 | 135.503 | 29.920 | 51.942 | 1.00 | 36.00 |
| | 1873 | H | SER | 213 | 136.366 | 29.279 | 49.173 | 1.00 | 25.00 |
| 10 | 1874 | HG | SER | 213 | 135.449 | 30.406 | 51.120 | 1.00 | 25.00 |
| | 1875 | N | ILE | 214 | 137.390 | 26.376 | 49.645 | 1.00 | 20.94 |
| | 1876 | CA | ILE | 214 | 137.701 | 24.958 | 49.502 | 1.00 | 20.03 |
| | 1877 | C | ILE | 214 | 138.869 | 24.617 | 48.591 | 1.00 | 20.98 |
| | 1878 | O | ILE | 214 | 139.914 | 24.174 | 49.065 | 1.00 | 23.05 |
| 15 | 1879 | CB | ILE | 214 | 136.463 | 24.144 | 49.041 | 1.00 | 20.03 |
| | 1880 | CG1 | ILE | 214 | 135.255 | 24.455 | 49.932 | 1.00 | 15.38 |
| | 1881 | CG2 | ILE | 214 | 136.778 | 22.640 | 49.046 | 1.00 | 14.86 |
| | 1882 | CD1 | ILE | 214 | 135.488 | 24.207 | 51.418 | 1.00 | 14.56 |
| | 1883 | H | ILE | 214 | 137.066 | 26.887 | 48.873 | 1.00 | 25.00 |
| 20 | 1884 | N | TYR | 215 | 138.696 | 24.823 | 47.289 | 1.00 | 18.70 |
| | 1885 | CA | TYR | 215 | 139.733 | 24.490 | 46.323 | 1.00 | 22.93 |
| | 1886 | C | TYR | 215 | 141.076 | 25.168 | 46.582 | 1.00 | 25.73 |
| | 1887 | O | TYR | 215 | 142.128 | 24.545 | 46.450 | 1.00 | 25.96 |
| | 1888 | CB | TYR | 215 | 139.258 | 24.777 | 44.899 | 1.00 | 19.89 |
| 25 | 1889 | CG | TYR | 215 | 139.859 | 23.834 | 43.884 | 1.00 | 17.39 |
| | 1890 | CD1 | TYR | 215 | 139.726 | 22.455 | 44.030 | 1.00 | 18.08 |
| | 1891 | CD2 | TYR | 215 | 140.557 | 24.315 | 42.782 | 1.00 | 19.17 |
| | 1892 | CE1 | TYR | 215 | 140.275 | 21.575 | 43.102 | 1.00 | 17.39 |
| | 1893 | CE2 | TYR | 215 | 141.113 | 23.445 | 41.843 | 1.00 | 16.77 |
| 30 | 1894 | CZ | TYR | 215 | 140.967 | 22.076 | 42.010 | 1.00 | 21.36 |
| | 1895 | OH | TYR | 215 | 141.517 | 21.212 | 41.088 | 1.00 | 25.91 |
| | 1896 | H | TYR | 215 | 137.858 | 25.217 | 46.973 | 1.00 | 25.00 |
| | 1897 | HH | TYR | 215 | 141.317 | 20.302 | 41.340 | 1.00 | 25.00 |
| | 1898 | N | ASP | 216 | 141.037 | 26.434 | 46.969 | 1.00 | 26.71 |
| 35 | 1899 | CA | ASP | 216 | 142.254 | 27.184 | 47.250 | 1.00 | 32.33 |
| | 1900 | C | ASP | 216 | 143.057 | 26.532 | 48.377 | 1.00 | 32.46 |
| | 1901 | O | ASP | 216 | 144.288 | 26.589 | 48.387 | 1.00 | 33.87 |
| | 1902 | CB | ASP | 216 | 141.895 | 28.621 | 47.636 | 1.00 | 35.77 |
| | 1903 | CG | ASP | 216 | 143.111 | 29.514 | 47.769 | 1.00 | 36.73 |
| 40 | 1904 | OD1 | ASP | 216 | 143.842 | 29.670 | 46.769 | 1.00 | 37.16 |
| | 1905 | OD2 | ASP | 216 | 143.327 | 30.062 | 48.871 | 1.00 | 41.08 |
| | 1906 | H | ASP | 216 | 140.170 | 26.885 | 447.054 | 1.00 | 25.00 |
| | 1907 | N | LYS | 217 | 142.350 | 25.910 | 49.316 | 1.00 | 31.70 |
| | 1908 | CA | LYS | 217 | 142.978 | 25.255 | 50.459 | 1.00 | 29.37 |
| 45 | 1909 | C | LYS | 217 | 143.134 | 23.745 | 50.269 | 1.00 | 30.32 |
| | 1910 | O | LYS | 217 | 143.506 | 23.029 | 51.200 | 1.00 | 31.00 |
| | 1911 | CB | LYS | 217 | 142.170 | 25.553 | 51.724 | 1.00 | 26.09 |
| | 1912 | CG | LYS | 217 | 142.062 | 27.033 | 52.017 | 1.00 | 27.73 |
| | 1913 | CD | LYS | 217 | 141.185 | 27.312 | 53.213 | 1.00 | 35.35 |
| 50 | 1914 | CE | LYS | 217 | 141.091 | 28.807 | 53.463 | 1.00 | 40.60 |
| | 1915 | NZ | LYS | 217 | 140.124 | 29.115 | 54.551 | 1.00 | 49.88 |
| | 1916 | H | LYS | 217 | 141.376 | 25.876 | 49.235 | 1.00 | 25.00 |

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|----|-------|------|-----|-----|---------|--------|--------|------|-------|
| | 1917 | 1HZ | LYS | 217 | 140.429 | 28.650 | 55.430 | 1.00 | 25.00 |
| | 1918 | 2HZ | LYS | 217 | 140.083 | 30.143 | 54.698 | 1.00 | 25.00 |
| | 1919 | 3HZ | LYS | 217 | 139.181 | 28.767 | 54.284 | 1.00 | 25.00 |
| | 1920 | N | GLU | 218 | 142.864 | 23.271 | 49.057 | 1.00 | 31.03 |
| 5 | 1921 | CA | GLU | 218 | 142.961 | 21.855 | 48.750 | 1.00 | 33.23 |
| | 1922 | C | GLU | 218 | 144.391 | 21.489 | 48.357 | 1.00 | 42.71 |
| | 1923 | O | GLU | 218 | 144.932 | 22.012 | 47.381 | 1.00 | 41.53 |
| | 1924 | CB | GLU | 218 | 141.983 | 21.492 | 47.626 | 1.00 | 32.79 |
| | 1925 | CG | GLU | 218 | 141.873 | 20.007 | 47.345 | 1.00 | 49.16 |
| 10 | 1926 | CD | GLU | 218 | 141.324 | 19.228 | 48.526 | 1.00 | 61.57 |
| | 1927 | OE1 | GLU | 218 | 140.147 | 19.456 | 48.886 | 1.00 | 66.99 |
| | 1928 | OE2 | GLU | 218 | 142.066 | 18.391 | 49.092 | 1.00 | 62.96 |
| | 1929 | H | GLU | 218 | 142.616 | 23.896 | 48.343 | 1.00 | 25.00 |
| | 1930 | N | GLN | 219 | 144.974 | 20.551 | 49.098 | 1.00 | 48.16 |
| 15 | 1931 | CA | GLN | 219 | 146.339 | 20.089 | 48.858 | 1.00 | 52.73 |
| | 1932 | C | GLN | 219 | 146.533 | 19.487 | 47.467 | 1.00 | 49.21 |
| | 1933 | O | GLN | 219 | 147.594 | 19.622 | 46.870 | 1.00 | 51.36 |
| | 1934 | CB | GLN | 219 | 146.733 | 19.063 | 49.929 | 1.00 | 62.56 |
| | 1935 | CG | GLN | 219 | 148.127 | 19.262 | 50.531 | 1.00 | 81.40 |
| 20 | 1936 | CD | GLN | 219 | 148.498 | 18.186 | 51.534 | 1.00 | 90.93 |
| | 1937 | OE1 | GLN | 219 | 148.863 | 17.072 | 51.156 | 1.00 | 97.11 |
| | 1938 | NE2 | GLN | 219 | 148.408 | 18.512 | 52.825 | 1.00 | 96.41 |
| | 1939 | H | GLN | 219 | 144.450 | 20.162 | 49.821 | 1.00 | 25.00 |
| | 1940 | 1HE2 | GLN | 219 | 148.113 | 19.389 | 53.115 | 1.00 | 25.00 |
| 25 | 1941 | 2HE2 | GLN | 219 | 148.656 | 17.793 | 53.455 | 1.00 | 25.00 |
| | 1942 | N | SER | 220 | 145.496 | 18.842 | 46.950 | 1.00 | 47.51 |
| | 1943 | CA | SER | 220 | 145.552 | 18.199 | 45.636 | 1.00 | 47.04 |
| | 1944 | C | SER | 220 | 144.945 | 19.020 | 44.487 | 1.00 | 45.29 |
| | 1945 | O | SER | 220 | 144.577 | 18.467 | 43.446 | 1.00 | 47.02 |
| 30 | 1946 | CB | SER | 220 | 144.862 | 16.833 | 45.713 | 1.00 | 51.73 |
| | 1947 | OG | SER | 220 | 143.585 | 16.948 | 46.327 | 1.00 | 55.26 |
| | 1948 | H | SER | 220 | 144.658 | 18.796 | 47.447 | 1.00 | 25.00 |
| | 1949 | HG | SER | 220 | 143.671 | 17.280 | 47.217 | 1.00 | 25.00 |
| | 1950 | N | LYS | 221 | 144.849 | 20.332 | 44.679 | 1.00 | 38.03 |
| 35 | 1951 | CA | LYS | 221 | 144.270 | 21.233 | 43.682 | 1.00 | 32.98 |
| | 1952 | C | LYS | 221 | 145.037 | 21.284 | 42.363 | 1.00 | 30.63 |
| | 1953 | O | LYS | 221 | 146.249 | 21.077 | 42.328 | 1.00 | 33.91 |
| | 1954 | CB | LYS | 221 | 144.206 | 22.649 | 44.255 | 1.00 | 33.08 |
| | 1955 | CG | LYS | 221 | 145.584 | 23.257 | 44.500 | 1.00 | 40.24 |
| 40 | 1956 | CD | LYS | 221 | 145.512 | 24.563 | 45.257 | 1.00 | 53.13 |
| | 19557 | CE | LYS | 221 | 146.902 | 25.093 | 45.561 | 1.00 | 55.90 |
| | 1958 | NZ | LYS | 221 | 146.843 | 26.358 | 46.344 | 1.00 | 67.32 |
| | 1959 | H | LYS | 221 | 145.198 | 20.720 | 45.508 | 1.00 | 25.00 |
| | 1960 | 1HZ | LYS | 221 | 146.350 | 26.191 | 47.244 | 1.00 | 25.00 |
| 45 | 1961 | 2HZ | LYS | 221 | 147.807 | 26.698 | 46.533 | 1.00 | 25.00 |
| | 1962 | 3HZ | LYS | 221 | 146.326 | 27.080 | 45.800 | 1.00 | 25.00 |
| | 1963 | N | ASN | 222 | 144.322 | 21.536 | 41.273 | 1.00 | 28.13 |
| | 1964 | CA | ASN | 222 | 144.958 | 21.675 | 39.970 | 1.00 | 25.27 |
| | 1965 | C | ASN | 222 | 145.154 | 23.174 | 39.816 | 1.00 | 30.00 |
| 50 | 1966 | O | ASN | 222 | 144.187 | 23.933 | 39.707 | 1.00 | 29.84 |
| | 1967 | CB | ASN | 222 | 144.077 | 21.149 | 38.843 | 1.00 | 22.73 |
| | 1968 | CG | ASN | 222 | 144.688 | 21.390 | 37.473 | 1.00 | 24.93 |

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|----|------|------|-----|-----|---------|--------|---------|------|-------|
| | 1969 | OD1 | ASN | 222 | 144.914 | 22.534 | 37.072 | 1.00 | 31.82 |
| | 1970 | ND2 | ASN | 222 | 144.973 | 20.317 | 36.755 | 1.00 | 23.78 |
| | 1971 | H | ASN | 222 | 143.353 | 21.640 | 41.343 | 1.00 | 25.00 |
| | 1972 | 1HD2 | ASN | 222 | 145.364 | 20.460 | 35.868 | 1.00 | 25.00 |
| 5 | 1973 | 2HD2 | ASN | 222 | 144.784 | 19.432 | 37.125 | 1.00 | 25.00 |
| | 1974 | N | ASN | 223 | 146.412 | 23.596 | 39.819 | 1.00 | 31.07 |
| | 1975 | CA | ASN | 223 | 146.759 | 25.009 | 39.726 | 1.00 | 26.94 |
| | 1976 | C | ASN | 223 | 146.273 | 25.730 | 38.477 | 1.00 | 25.82 |
| | 1977 | O | ASN | 223 | 145.933 | 26.910 | 38.538 | 1.00 | 27.88 |
| 10 | 1978 | CB | ASN | 223 | 148.261 | 25.185 | 39.915 | 1.00 | 23.98 |
| | 1979 | CG | ASN | 223 | 148.739 | 24.633 | 41.242 | 1.00 | 28.15 |
| | 1980 | OD1 | ASN | 223 | 148.586 | 25.271 | 42.281 | 1.00 | 30.20 |
| | 1981 | ND2 | ASN | 223 | 149.291 | 23.423 | 41.219 | 1.00 | 25.49 |
| | 1982 | H | ASN | 223 | 147.118 | 22.925 | 39.901 | 1.00 | 25.00 |
| 15 | 1983 | 1HD2 | ASN | 223 | 149.595 | 23.063 | 42.082 | 1.00 | 25.00 |
| | 1984 | 2HD2 | ASN | 223 | 149.377 | 22.938 | 40.382 | 1.00 | 25.00 |
| | 1985 | N | VAL | 224 | 146.224 | 25.036 | 37.346 | 1.00 | 24.73 |
| | 1986 | CA | VAL | 224 | 145.743 | 25.667 | 36.124 | 1.00 | 27.15 |
| | 1987 | C | VAL | 224 | 144.263 | 26.026 | 36.304 | 1.00 | 28.87 |
| 20 | 1988 | O | VAL | 224 | 143.852 | 27.150 | 36.019 | 1.00 | 29.97 |
| | 1989 | CB | VAL | 224 | 145.914 | 24.742 | 34.900 | 1.00 | 31.17 |
| | 1990 | CG1 | VAL | 224 | 145.359 | 25.404 | 33.651 | 1.00 | 30.27 |
| | 1991 | CG2 | VAL | 224 | 147.382 | 24.400 | 34.707 | 1.00 | 30.28 |
| | 1992 | H | VAL | 224 | 146.488 | 24.096 | 37.329 | 1.00 | 25.00 |
| 25 | 1993 | N | LEU | 225 | 143.486 | 25.089 | 36.843 | 1.00 | 25.78 |
| | 1994 | CA | LEU | 225 | 142.057 | 25.303 | 37.069 | 1.00 | 25.90 |
| | 1995 | C | LEU | 225 | 141.792 | 26.380 | 38.125 | 1.00 | 26.51 |
| | 1996 | O | LEU | 225 | 140.900 | 27.214 | 37.956 | 1.00 | 26.55 |
| | 1997 | CB | LEU | 225 | 141.366 | 23.991 | 37.463 | 1.00 | 20.07 |
| 30 | 1998 | CG | LEU | 225 | 141.398 | 22.848 | 36.441 | 1.00 | 21.81 |
| | 1999 | CD1 | LEU | 225 | 140.664 | 21.638 | 36.991 | 1.00 | 10.56 |
| | 2000 | CD2 | LEU | 225 | 140.780 | 23.295 | 35.126 | 1.00 | 19.02 |
| | 2001 | H | LEU | 225 | 143.883 | 24.229 | 37.092 | 1.00 | 25.00 |
| | 2002 | N | LEU | 226 | 142.566 | 26.369 | 39.207 | 1.00 | 22.12 |
| 35 | 2003 | CA | LEU | 226 | 142.400 | 27.367 | 40.261 | 1.00 | 27.39 |
| | 2004 | C | LEU | 226 | 142.724 | 28.775 | 39.743 | 1.00 | 28.78 |
| | 2005 | O | LEU | 226 | 141.967 | 29.720 | 39.969 | 1.00 | 34.36 |
| | 2006 | CB | LEU | 226 | 143.282 | 27.033 | 41.468 | 1.00 | 25.60 |
| | 2007 | CG | LEU | 226 | 143.170 | 27.984 | 42.6665 | 1.00 | 26.39 |
| 40 | 2008 | CD1 | LEU | 226 | 141.731 | 28.037 | 43.183 | 1.00 | 20.17 |
| | 2009 | CD2 | LEU | 226 | 144.110 | 27.532 | 43.763 | 1.00 | 26.04 |
| | 2010 | H | LEU | 226 | 143.249 | 25.673 | 39.298 | 1.00 | 25.00 |
| | 2011 | N | ARG | 227 | 143.842 | 28.904 | 39.036 | 1.00 | 28.64 |
| | 2012 | CA | ARG | 227 | 144.270 | 30.183 | 38.473 | 1.00 | 30.51 |
| 45 | 2013 | C | ARG | 227 | 143.186 | 30.688 | 37.508 | 1.00 | 29.19 |
| | 2014 | O | ARG | 227 | 142.770 | 31.849 | 37.567 | 1.00 | 25.86 |
| | 2015 | CB | ARG | 227 | 145.607 | 29.989 | 37.742 | 1.00 | 30.51 |
| | 2016 | CG | ARG | 227 | 146.171 | 31.215 | 37.037 | 1.00 | 32.00 |
| | 2017 | CD | ARG | 227 | 146.883 | 32.162 | 37.981 | 1.00 | 35.49 |
| 50 | 2018 | NE | ARG | 227 | 147.414 | 33.314 | 37.256 | 1.00 | 34.46 |
| | 2019 | CZ | ARG | 227 | 147.799 | 34.454 | 37.822 | 1.00 | 32.62 |
| | 2020 | NH1 | ARG | 227 | 147.727 | 34.611 | 39.136 | 1.00 | 33.39 |

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|----|------|------|-----|-----|---------|--------|--------|------|-------|
| | 2021 | NH2 | ARG | 227 | 148.214 | 35.460 | 37.066 | 1.00 | 35.87 |
| | 2022 | H | ARG | 227 | 144.402 | 28.114 | 38.884 | 1.00 | 25.00 |
| | 2023 | HE | ARG | 227 | 147.480 | 33.245 | 36.292 | 1.00 | 25.00 |
| | 2024 | 1HH1 | ARG | 227 | 147.381 | 33.871 | 39.712 | 1.00 | 25.00 |
| 5 | 2025 | 2HH1 | ARG | 227 | 148.020 | 35.470 | 39.554 | 1.00 | 25.00 |
| | 2026 | 1HH2 | ARG | 227 | 148.236 | 35.359 | 36.073 | 1.00 | 25.00 |
| | 2027 | 2HH2 | ARG | 227 | 148.505 | 36.315 | 37.491 | 1.00 | 25.00 |
| | 2028 | N | PHE | 228 | 142.723 | 29.788 | 36.645 | 1.00 | 28.49 |
| | 2029 | CA | PHE | 228 | 141.678 | 30.063 | 35.656 | 1.00 | 30.24 |
| 10 | 2030 | C | PHE | 228 | 140.411 | 30.575 | 36.369 | 1.00 | 29.56 |
| | 2031 | O | PHE | 228 | 139.909 | 31.662 | 36.068 | 1.00 | 31.17 |
| | 2032 | CB | PHE | 228 | 141.394 | 28.752 | 34.892 | 1.00 | 32.31 |
| | 2033 | CG | PHE | 228 | 140.441 | 28.879 | 33.721 | 1.00 | 30.15 |
| | 2034 | CD1 | PHE | 228 | 139.889 | 30.103 | 33.348 | 1.00 | 29.90 |
| 15 | 2035 | CD2 | PHE | 228 | 140.084 | 27.740 | 32.999 | 1.00 | 24.53 |
| | 2036 | CE1 | PHE | 228 | 138.994 | 30.186 | 32.277 | 1.00 | 28.21 |
| | 2037 | CE2 | PHE | 228 | 139.193 | 27.811 | 31.930 | 1.00 | 23.61 |
| | 2038 | CZ | PHE | 228 | 138.646 | 29.036 | 31.568 | 1.00 | 29.31 |
| | 2039 | H | PHE | 228 | 143.108 | 28.886 | 36.672 | 1.00 | 25.00 |
| 20 | 2040 | N | ALA | 229 | 139.935 | 29.809 | 37.344 | 1.00 | 25.42 |
| | 2041 | CA | ALA | 229 | 138.737 | 30.156 | 38.099 | 1.00 | 25.11 |
| | 2042 | C | ALA | 229 | 138.808 | 31.533 | 38.764 | 1.00 | 29.20 |
| | 2043 | O | ALA | 229 | 137.847 | 32.310 | 38.703 | 1.00 | 26.99 |
| | 2044 | CB | ALA | 229 | 138.456 | 29.085 | 39.135 | 1.00 | 20.89 |
| 25 | 2045 | H | ALA | 229 | 140.406 | 28.982 | 37.565 | 1.00 | 25.00 |
| | 2046 | N | LYS | 230 | 139.944 | 31.838 | 39.389 | 1.00 | 29.21 |
| | 2047 | CA | LYS | 230 | 140.127 | 33.121 | 40.068 | 1.00 | 29.75 |
| | 2048 | C | LYS | 230 | 140.100 | 34.306 | 39.109 | 1.00 | 30.11 |
| | 2049 | O | LYS | 230 | 139.405 | 35.298 | 39.350 | 1.00 | 30.69 |
| 30 | 2050 | CB | LYS | 230 | 141.434 | 33.136 | 40.866 | 1.00 | 30.27 |
| | 2051 | CG | LYS | 230 | 141.422 | 32.247 | 42.100 | 1.00 | 29.79 |
| | 2052 | CD | LYS | 230 | 142.686 | 32.430 | 42.923 | 1.00 | 24.40 |
| | 2053 | CE | LYS | 230 | 142.595 | 31.664 | 44.227 | 1.00 | 29.55 |
| | 2054 | NZ | LYS | 230 | 143.790 | 31.883 | 45.079 | 1.00 | 36.37 |
| 35 | 2055 | H | LYS | 230 | 140.676 | 31.183 | 39.394 | 1.00 | 25.00 |
| | 2056 | 1HZ | LYS | 230 | 143.881 | 32.896 | 45.296 | 1.00 | 25.00 |
| | 2057 | 2HZ | LYS | 230 | 143.689 | 31.356 | 45.965 | 1.00 | 25.00 |
| | 2058 | 33HZ | LYS | 230 | 144.640 | 31.560 | 44.573 | 1.00 | 25.00 |
| | 2059 | N | LEU | 231 | 140.852 | 34.201 | 38.016 | 1.00 | 31.56 |
| 40 | 2060 | CA | LEU | 231 | 140.911 | 35.275 | 37.032 | 1.00 | 30.17 |
| | 2061 | C | LEU | 231 | 139.549 | 35.506 | 36.394 | 1.00 | 30.20 |
| | 2062 | O | LEU | 231 | 139.085 | 36.645 | 36.299 | 1.00 | 26.72 |
| | 2063 | CB | LEU | 231 | 141.941 | 34.959 | 35.941 | 1.00 | 29.21 |
| | 2064 | CG | LEU | 231 | 143.408 | 34.790 | 36.340 | 1.00 | 26.11 |
| 45 | 2065 | CD1 | LEU | 231 | 144.232 | 34.631 | 35.077 | 1.00 | 22.49 |
| | 2066 | CD2 | LEU | 231 | 143.890 | 35.990 | 37.139 | 1.00 | 22.48 |
| | 2067 | H | LEU | 231 | 141.374 | 33.380 | 37.869 | 1.00 | 25.00 |
| | 2068 | N | ASP | 232 | 138.898 | 34.417 | 35.995 | 1.00 | 29.28 |
| | 2069 | CA | ASP | 232 | 137.593 | 34.490 | 35.351 | 1.00 | 28.41 |
| 50 | 2070 | C | ASP | 232 | 136.549 | 35.149 | 36.247 | 1.00 | 25.56 |
| | 2071 | O | ASP | 232 | 135.820 | 36.044 | 35.813 | 1.00 | 25.21 |
| | 2072 | CB | ASP | 232 | 137.131 | 33.097 | 34.932 | 1.00 | 26.05 |

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|----|------|------|-----|------|----------|--------|--------|------|-------|
| | 2073 | CG | ASP | 232 | 136.143 | 33.143 | 33.793 | 1.00 | 33.93 |
| | 2074 | OD1 | ASP | 232 | 136.587 | 33.188 | 32.627 | 1.00 | 32.45 |
| | 2075 | OD2 | ASP | 232 | 134.927 | 33.157 | 34.060 | 1.00 | 29.97 |
| | 2076 | H | ASP | 232 | 139.310 | 33.539 | 36.141 | 1.00 | 25.00 |
| 5 | 2077 | N | PHE | 233 | 136.510 | 34.730 | 37.507 | 1.00 | 24.45 |
| | 2078 | CA | PHE | 233 | 135.569 | 35.286 | 38.466 | 1.00 | 22.77 |
| | 2079 | C | PHE | 233 | 135.788 | 36.788 | 38.603 | 1.00 | 28.10 |
| | 2080 | O | PHE | 233 | 134.835 | 37.568 | 38.516 | 1.00 | 31.99 |
| | 2081 | CB | PHE | 233 | 135.732 | 34.605 | 39.831 | 1.00 | 19.36 |
| 10 | 2082 | CG | PHE | 233 | 134.714 | 35.035 | 40.854 | 1.00 | 22.51 |
| | 2083 | CD1 | PHE | 233 | 1344.857 | 36.241 | 41.540 | 1.00 | 22.18 |
| | 2084 | CD2 | PHE | 233 | 133.604 | 34.237 | 41.127 | 1.00 | 23.90 |
| | 2085 | CE1 | PHE | 233 | 133.906 | 36.646 | 42.481 | 1.00 | 26.05 |
| | 2086 | CE2 | PHE | 233 | 132.650 | 34.631 | 42.065 | 1.00 | 23.08 |
| 15 | 2087 | CZ | PHE | 233 | 132.801 | 35.839 | 42.743 | 1.00 | 24.51 |
| | 2088 | H | PHE | 233 | 137.126 | 34.022 | 37.802 | 1.00 | 25.00 |
| | 2089 | N | ASN | 234 | 137.044 | 37.189 | 38.801 | 1.00 | 28.39 |
| | 2090 | CA | ASN | 234 | 137.393 | 38.602 | 38.965 | 1.00 | 28.37 |
| | 2091 | C | ASN | 234 | 137.079 | 39.446 | 37.743 | 1.00 | 27.25 |
| 20 | 2092 | O | ASN | 234 | 136.606 | 40.575 | 37.868 | 1.00 | 32.70 |
| | 2093 | CB | ASN | 234 | 138.867 | 38.762 | 39.342 | 1.00 | 27.32 |
| | 2094 | CG | ASN | 234 | 139.152 | 38.353 | 40.776 | 1.00 | 30.63 |
| | 2095 | OD1 | ASN | 234 | 138.242 | 38.219 | 41.595 | 1.00 | 29.34 |
| | 2096 | ND2 | ASN | 234 | 140.426 | 38.166 | 41.092 | 1.00 | 37.28 |
| 25 | 2097 | H | ASN | 234 | 137.753 | 36.513 | 38.851 | 1.00 | 25.00 |
| | 2098 | 1HD2 | ASN | 234 | 140.628 | 37.901 | 42.015 | 1.00 | 25.00 |
| | 2099 | 2HD2 | ASN | 234 | 141.114 | 38.292 | 40.408 | 1.00 | 25.00 |
| | 2100 | N | LEU | 235 | 137.339 | 38.902 | 36.561 | 1.00 | 28.66 |
| | 2101 | CA | LEU | 235 | 137.059 | 39.616 | 35.321 | 1.00 | 29.93 |
| 30 | 2102 | C | LEU | 235 | 135.551 | 39.830 | 35.167 | 1.00 | 30.84 |
| | 2103 | O | LEU | 235 | 135.106 | 40.949 | 34.908 | 1.00 | 31.89 |
| | 2104 | CB | LEU | 235 | 137.625 | 38.852 | 34.119 | 1.00 | 29.05 |
| | 2105 | CG | LEU | 235 | 137.476 | 39.509 | 32.742 | 1.00 | 30.21 |
| | 2106 | CD1 | LEU | 235 | 138.045 | 40.922 | 32.769 | 1.00 | 29.02 |
| 35 | 2107 | CD2 | LEU | 235 | 138.173 | 38.667 | 31.684 | 1.00 | 31.45 |
| | 2108 | H | LEU | 235 | 137.721 | 38.001 | 36.525 | 1.00 | 25.00 |
| | 2109 | N | LEU | 236 | 134.766 | 38.769 | 35.352 | 1.00 | 29.90 |
| | 2110 | CA | LEU | 236 | 133.311 | 38.875 | 35.245 | 1.00 | 28.94 |
| | 2111 | C | LEU | 236 | 132.774 | 39.874 | 36.263 | 1.00 | 28.31 |
| 40 | 2112 | O | LEU | 236 | 131.833 | 40.623 | 35.979 | 1.00 | 29.04 |
| | 2113 | CB | LEU | 236 | 132.632 | 37.518 | 35.463 | 1.00 | 26.96 |
| | 2114 | CG | LEU | 236 | 132.722 | 36.463 | 34.359 | 1.00 | 32.49 |
| | 2115 | CD1 | LEU | 236 | 131.797 | 35.299 | 34.694 | 1.00 | 28.63 |
| | 2116 | CD2 | LEU | 236 | 132.326 | 37.068 | 33.026 | 1.00 | 30.07 |
| 45 | 2117 | H | LEU | 236 | 135.173 | 37.900 | 35.561 | 1.00 | 25.00 |
| | 2118 | N | GLN | 237 | 133.362 | 39.870 | 37.454 | 1.00 | 25.46 |
| | 2119 | CA | GLN | 237 | 132.953 | 40.777 | 38.521 | 1.00 | 25.58 |
| | 2120 | C | GLN | 237 | 133.059 | 42.231 | 38.062 | 1.00 | 27.92 |
| | 2121 | O | GLN | 2337 | 132.201 | 43.054 | 38.387 | 1.00 | 29.65 |
| 50 | 2122 | CB | GLN | 237 | 133.807 | 40.549 | 39.769 | 1.00 | 20.55 |
| | 2123 | CG | GLN | 237 | 133.342 | 41.314 | 40.993 | 1.00 | 23.60 |
| | 2124 | CD | GLN | 237 | 134.216 | 41.046 | 42.197 | 1.00 | 31.25 |

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|----|------|------|-----|-----|---------|--------|--------|------|-------|
| | 2125 | OE1 | GLN | 237 | 135.435 | 41.196 | 42.134 | 1.00 | 31.93 |
| | 2126 | NE2 | GLN | 237 | 133.602 | 40.634 | 43.298 | 1.00 | 28.03 |
| | 2127 | H | GLN | 237 | 134.094 | 39.237 | 37.625 | 1.00 | 25.00 |
| | 2128 | 1HE2 | GLN | 237 | 134.156 | 40.446 | 44.081 | 1.00 | 25.00 |
| 5 | 2129 | 2HE2 | GLN | 237 | 132.635 | 40.519 | 43.287 | 1.00 | 25.00 |
| | 2130 | N | MET | 238 | 134.096 | 42.537 | 37.286 | 1.00 | 28.91 |
| | 2131 | CA | MET | 238 | 134.288 | 43.888 | 36.776 | 1.00 | 33.08 |
| | 2132 | C | MET | 238 | 133.084 | 44.282 | 35.924 | 1.00 | 33.53 |
| | 2133 | O | MET | 238 | 132.562 | 45.391 | 36.049 | 1.00 | 37.31 |
| 10 | 2134 | CB | MET | 238 | 135.573 | 43.976 | 35.954 | 1.00 | 32.86 |
| | 2135 | CG | MET | 238 | 136.836 | 43.837 | 36.782 | 1.00 | 39.06 |
| | 2136 | SD | MET | 238 | 138.318 | 43.815 | 35.763 | 1.00 | 43.74 |
| | 2137 | CE | MET | 238 | 139.508 | 43.186 | 36.929 | 1.00 | 46.28 |
| | 2138 | H | MET | 238 | 134.751 | 41.842 | 37.055 | 1.00 | 25.00 |
| 15 | 2139 | N | LEU | 239 | 132.624 | 43.356 | 35.087 | 1.00 | 31.84 |
| | 2140 | CA | LEU | 239 | 131.465 | 43.599 | 34.233 | 1.00 | 30.89 |
| | 2141 | C | LEU | 239 | 130.219 | 43.801 | 35.097 | 1.00 | 28.36 |
| | 2142 | O | LEU | 239 | 129.450 | 44.742 | 34.885 | 1.00 | 32.90 |
| | 2143 | CB | LEU | 239 | 131.255 | 42.427 | 33.271 | 1.00 | 29.61 |
| 20 | 2144 | CG | LEU | 239 | 129.969 | 42.432 | 32.436 | 1.00 | 29.85 |
| | 2145 | CD1 | LEU | 239 | 129.929 | 43.636 | 31.499 | 1.00 | 25.22 |
| | 2146 | CD2 | LEU | 239 | 129.870 | 41.138 | 31.649 | 1.00 | 26.65 |
| | 2147 | H | LEU | 239 | 133.084 | 42.491 | 35.043 | 1.00 | 25.00 |
| | 2148 | N | HIS | 240 | 130.042 | 42.942 | 36.095 | 1.00 | 25.85 |
| 25 | 2149 | CA | HIS | 240 | 128.891 | 43.042 | 36.990 | 1.00 | 28.32 |
| | 2150 | C | HIS | 240 | 128.885 | 44.406 | 37.671 | 1.00 | 30.20 |
| | 2151 | O | HIS | 240 | 127.824 | 44.974 | 37.940 | 1.00 | 30.10 |
| | 2152 | CB | HIS | 240 | 128.925 | 41.926 | 38.036 | 1.00 | 25.55 |
| | 2153 | CG | HIS | 240 | 128.881 | 40.545 | 37.448 | 1.00 | 24.20 |
| 30 | 2154 | ND1 | HIS | 240 | 129.449 | 39.455 | 38.058 | 1.00 | 25.29 |
| | 2155 | CD2 | HIS | 240 | 128.358 | 40.103 | 36.283 | 1.00 | 21.44 |
| | 2156 | CE1 | HIS | 240 | 129.289 | 38.394 | 37.302 | 1.00 | 27.58 |
| | 2157 | NE2 | HIS | 240 | 128.627 | 38.750 | 36.209 | 1.00 | 21.74 |
| | 2158 | H | HIS | 240 | 130.713 | 42.244 | 36.233 | 1.00 | 25.00 |
| 35 | 2159 | HD11 | HIS | 240 | 129.918 | 39.455 | 38.924 | 1.00 | 25.00 |
| | 2160 | HE2 | HIS | 240 | 128.362 | 38.151 | 35.470 | 1.00 | 25.00 |
| | 2161 | N | LYS | 241 | 130.079 | 44.926 | 37.935 | 1.00 | 34.60 |
| | 2162 | CA | LYS | 241 | 130.239 | 46.230 | 38.563 | 1.00 | 32.03 |
| | 2163 | C | LYS | 241 | 129.855 | 47.374 | 37.613 | 1.00 | 31.99 |
| 40 | 2164 | O | LYS | 241 | 129.280 | 48.374 | 38.045 | 1.00 | 29.66 |
| | 2165 | CB | LYS | 241 | 131.675 | 46.391 | 39.072 | 1.00 | 32.10 |
| | 2166 | CG | LYS | 241 | 131.984 | 45.614 | 40.356 | 1.00 | 34.40 |
| | 2167 | CD | LYS | 241 | 133.447 | 45.807 | 40.758 | 1.00 | 41.19 |
| | 2168 | CE | LYS | 241 | 133.701 | 45.417 | 42.208 | 1.00 | 49.51 |
| 45 | 2169 | NZ | LYS | 241 | 135.044 | 45.881 | 42.698 | 1.00 | 56.06 |
| | 2170 | H | LYS | 241 | 130.875 | 44.403 | 37.703 | 1.00 | 25.00 |
| | 2171 | 1HZ | LYS | 241 | 135.111 | 46.916 | 42.625 | 1.00 | 25.00 |
| | 2172 | 2HZ | LYS | 241 | 135.179 | 45.610 | 43.698 | 1.00 | 25.00 |
| | 2173 | 3HZ | LYS | 241 | 135.803 | 45.446 | 42.135 | 1.00 | 25.00 |
| 50 | 2174 | N | GLN | 242 | 130.121 | 47.201 | 36.316 | 1.00 | 34.13 |
| | 2175 | CA | GLN | 242 | 129.799 | 48.211 | 35.303 | 1.00 | 38.39 |
| | 2176 | C | GLN | 242 | 128.288 | 48.278 | 35.161 | 1.00 | 39.98 |

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|----|------|------|-----|-----|----------|--------|--------|------|-------|
| | 2177 | O | GLN | 242 | 127.702 | 49.353 | 34.990 | 1.00 | 45.19 |
| | 2178 | CB | GLN | 242 | 130.376 | 47.827 | 33.942 | 1.00 | 42.52 |
| | 2179 | CG | GLN | 242 | 131.883 | 47.683 | 33.920 | 1.00 | 60.88 |
| | 2180 | CD | GLN | 242 | 132.417 | 47.252 | 32.574 | 1.00 | 69.61 |
| 5 | 2181 | OE1 | GLN | 242 | 131.663 | 47.052 | 31.620 | 1.00 | 75.13 |
| | 2182 | NE2 | GLN | 242 | 133.730 | 47.102 | 32.488 | 1.00 | 78.40 |
| | 2183 | H | GLN | 242 | 130.490 | 46.358 | 35.996 | 1.00 | 25.00 |
| | 2184 | 1HE2 | GLN | 242 | 134.0772 | 46.820 | 31.621 | 1.00 | 25.00 |
| | 2185 | 2HE2 | GLN | 242 | 134.282 | 47.272 | 33.272 | 1.00 | 25.00 |
| 10 | 2186 | N | GLU | 243 | 127.674 | 47.105 | 35.219 | 1.00 | 33.89 |
| | 2187 | CA | GLU | 243 | 126.233 | 46.975 | 35.107 | 1.00 | 28.66 |
| | 2188 | C | GLU | 243 | 125.568 | 47.591 | 36.325 | 1.00 | 28.27 |
| | 2189 | O | GLU | 243 | 124.635 | 48.381 | 36.193 | 1.00 | 32.26 |
| | 2190 | CB | GLU | 243 | 125.857 | 45.505 | 34.982 | 1.00 | 25.09 |
| 15 | 2191 | CG | GLU | 243 | 126.416 | 44.820 | 33.741 | 1.00 | 24.03 |
| | 2192 | CD | GLU | 243 | 126.182 | 43.329 | 33.738 | 1.00 | 26.58 |
| | 2193 | OE1 | GLU | 243 | 125.633 | 42.810 | 34.726 | 1.00 | 24.63 |
| | 2194 | OE2 | GLU | 243 | 126.556 | 42.665 | 32.750 | 1.00 | 29.69 |
| | 2195 | H | GLU | 243 | 128.248 | 46.333 | 35.341 | 1.00 | 25.00 |
| 20 | 2196 | N | LEU | 244 | 126.078 | 47.267 | 37.508 | 1.00 | 24.94 |
| | 2197 | CA | LEU | 244 | 125.522 | 47.798 | 38.745 | 1.00 | 30.48 |
| | 2198 | C | LEU | 244 | 125.635 | 49.324 | 38.766 | 1.00 | 36.45 |
| | 2199 | O | LEU | 244 | 124.700 | 50.021 | 39.163 | 1.00 | 35.07 |
| | 2200 | CB | LEU | 244 | 126.233 | 47.185 | 39.957 | 1.00 | 28.96 |
| 25 | 2201 | CG | LEU | 244 | 125.765 | 47.658 | 41.339 | 1.00 | 29.10 |
| | 2202 | CD1 | LEU | 244 | 124.249 | 47.527 | 41.484 | 1.00 | 25.23 |
| | 2203 | CD2 | LEU | 244 | 126.464 | 46.859 | 42.423 | 1.00 | 27.57 |
| | 2204 | H | LEU | 244 | 126.855 | 46.662 | 37.535 | 1.00 | 25.00 |
| | 2205 | N | ALA | 245 | 126.778 | 49.832 | 38.318 | 1.00 | 37.15 |
| 30 | 2206 | CA | ALA | 245 | 127.023 | 51.268 | 38.270 | 1.00 | 38.62 |
| | 2207 | C | ALA | 245 | 126.030 | 51.937 | 37.325 | 1.00 | 39.57 |
| | 2208 | O | ALA | 245 | 125.352 | 52.902 | 37.692 | 1.00 | 43.21 |
| | 2209 | CB | ALA | 245 | 128.452 | 51.539 | 37.802 | 1.00 | 35.23 |
| | 2210 | H | ALA | 245 | 127.477 | 49.215 | 38.032 | 1.00 | 25.00 |
| 35 | 2211 | N | GLN | 246 | 125.920 | 51.380 | 36.123 | 1.00 | 35.82 |
| | 2212 | CA | GLN | 246 | 125.025 | 51.888 | 35.086 | 1.00 | 40.78 |
| | 2213 | C | GLN | 246 | 123.577 | 51.989 | 35.566 | 1.00 | 43.61 |
| | 2214 | O | GLN | 246 | 122.907 | 53.016 | 35.404 | 1.00 | 43.37 |
| | 2215 | CB | GLN | 246 | 125.088 | 50.963 | 33.872 | 1.00 | 42.45 |
| 40 | 2216 | CG | GLN | 246 | 124.151 | 51.350 | 32.733 | 1.00 | 59.73 |
| | 2217 | CD | GLN | 246 | 124.146 | 50.338 | 31.610 | 1.00 | 65.77 |
| | 2218 | OE1 | GLN | 246 | 125.149 | 49.663 | 31.357 | 1.00 | 67.95 |
| | 2219 | NE2 | GLN | 246 | 123.009 | 50.223 | 30.920 | 1.00 | 66.48 |
| | 2220 | H | GLN | 246 | 126.450 | 50.576 | 35.964 | 1.00 | 25.00 |
| 45 | 2221 | 1HE2 | GLN | 246 | 123.038 | 49.559 | 30.198 | 1.00 | 25.00 |
| | 2222 | 2HE2 | GLN | 246 | 122.232 | 50.763 | 31.132 | 1.00 | 25.00 |
| | 2223 | N | VAL | 247 | 123.115 | 50.916 | 36.185 | 1.00 | 39.07 |
| | 2224 | CA | VAL | 247 | 121.762 | 50.830 | 36.692 | 1.00 | 37.02 |
| | 2225 | C | VAL | 247 | 121.538 | 51.732 | 37.908 | 1.00 | 40.33 |
| 50 | 2226 | O | VAL | 247 | 120.435 | 52.248 | 38.106 | 1.00 | 39.92 |
| | 2227 | CB | VAL | 247 | 121.387 | 49.341 | 36.946 | 1.00 | 35.95 |
| | 2228 | CG1 | VAL | 247 | 120.417 | 49.201 | 38.091 | 1.00 | 37.82 |

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|----|------|------|------|-----|---------|--------|---------|------|-------|
| | 2229 | CG2 | VAL | 247 | 120.794 | 48.754 | 35.686 | 1.00 | 32.90 |
| | 2230 | H | VAL | 247 | 123.730 | 50.170 | 36.340 | 1.00 | 25.00 |
| | 2231 | N | SER | 248 | 122.579 | 51.926 | 38.715 | 1.00 | 44.51 |
| | 2232 | CA | SER | 248 | 122.483 | 52.798 | 39.887 | 1.00 | 46.80 |
| 5 | 2233 | C | SER | 248 | 122.250 | 54.234 | 39.410 | 1.00 | 47.29 |
| | 2234 | O | SER | 248 | 121.454 | 54.976 | 39.997 | 1.00 | 46.67 |
| | 2235 | CB | SER | 248 | 123.759 | 52.727 | 40.726 | 1.00 | 44.77 |
| | 2236 | OG | SER | 248 | 123.859 | 51.479 | 41.381 | 1.00 | 45.74 |
| | 2237 | H | SER | 248 | 123.423 | 51.465 | 38.531 | 1.00 | 25.00 |
| 10 | 2238 | HG | SER | 248 | 123.876 | 50.777 | 40.722 | 1.00 | 25.00 |
| | 2239 | N | ARG | 249 | 122.938 | 54.615 | 38.334 | 1.00 | 44.35 |
| | 2240 | CA | ARG | 249 | 122.789 | 55.943 | 37.750 | 1.00 | 48.22 |
| | 2241 | C | ARG | 249 | 121.354 | 56.097 | 37.256 | 1.00 | 47.00 |
| | 2242 | O | ARG | 249 | 120.710 | 57.119 | 37.504 | 1.00 | 47.12 |
| 15 | 2243 | CB | ARG | 249 | 123.785 | 56.147 | 36.604 | 1.00 | 52.69 |
| | 2244 | CG | ARG | 249 | 125.165 | 56.590 | 37.075 | 1.00 | 66.38 |
| | 2245 | CD | ARG | 249 | 126.154 | 56.712 | 35.924 | 1.00 | 73.20 |
| | 2246 | NE | ARG | 249 | 126.919 | 55.484 | 35.712 | 1.00 | 75.40 |
| | 2247 | CZ | ARG | 249 | 126.922 | 54.778 | 334.584 | 1.00 | 77.33 |
| 20 | 2248 | NH1 | ARG | 249 | 126.194 | 55.165 | 33.542 | 1.00 | 74.66 |
| | 2249 | NH2 | ARG | 249 | 127.669 | 53.686 | 34.493 | 1.00 | 83.65 |
| | 2250 | H | ARG | 249 | 123.579 | 53.986 | 37.936 | 1.00 | 25.00 |
| | 2251 | HE | ARG | 249 | 127.471 | 55.153 | 36.453 | 1.00 | 25.00 |
| | 2252 | 1HH1 | ARG | 249 | 125.633 | 55.990 | 33.598 | 1.00 | 25.00 |
| 25 | 2253 | 2HH1 | ARG | 249 | 126.203 | 54.625 | 32.700 | 1.00 | 25.00 |
| | 2254 | 1HH2 | ARG | 249 | 128.229 | 53.396 | 35.269 | 1.00 | 25.00 |
| | 2255 | 2HH2 | ARG | 249 | 127.675 | 53.153 | 33.646 | 1.00 | 25.00 |
| | 2256 | N | TRP | 250 | 120.848 | 55.053 | 36.603 | 1.00 | 46.33 |
| | 2257 | CA | TRP | 250 | 119.480 | 55.024 | 36.092 | 1.00 | 43.84 |
| 30 | 2258 | C | TRP | 250 | 118.488 | 55.311 | 37.230 | 1.00 | 46.38 |
| | 2259 | O | TRP | 250 | 117.566 | 56.118 | 37.075 | 1.00 | 44.72 |
| | 2260 | CB | TRRP | 250 | 119.201 | 53.652 | 35.456 | 1.00 | 38.48 |
| | 2261 | CG | TRP | 250 | 117.747 | 53.324 | 35.232 | 1.00 | 37.37 |
| | 2262 | CD1 | TRP | 250 | 116.986 | 53.661 | 34.150 | 1.00 | 33.31 |
| 35 | 2263 | CD2 | TRP | 250 | 116.891 | 52.569 | 36.105 | 1.00 | 36.85 |
| | 2264 | NE1 | TRP | 250 | 115.713 | 53.164 | 34.293 | 1.00 | 34.01 |
| | 2265 | CE2 | TRP | 250 | 115.626 | 52.490 | 35.483 | 1.00 | 36.82 |
| | 2266 | CE3 | TRP | 250 | 117.070 | 51.952 | 37.352 | 1.00 | 34.91 |
| | 2267 | CZ2 | TRP | 250 | 114.543 | 51.816 | 36.065 | 1.00 | 39.04 |
| 40 | 2268 | CZ3 | TRP | 250 | 115.992 | 51.281 | 37.932 | 1.00 | 39.64 |
| | 2269 | CH2 | TRP | 250 | 114.746 | 51.220 | 37.286 | 1.00 | 39.49 |
| | 2270 | H | TRP | 250 | 121.423 | 54.272 | 36.448 | 1.00 | 25.00 |
| | 2271 | HE1 | TRP | 250 | 114.984 | 53.281 | 33.650 | 1.00 | 25.00 |
| | 2272 | N | TRP | 251 | 118.718 | 54.683 | 38.382 | 1.00 | 46.65 |
| 45 | 2273 | CA | TRP | 251 | 117.859 | 54.851 | 39.551 | 1.00 | 54.20 |
| | 2274 | C | TRP | 251 | 117.864 | 56.279 | 40.089 | 1.00 | 59.43 |
| | 2275 | O | TRP | 251 | 116.814 | 56.823 | 40.445 | 1.00 | 62.13 |
| | 2276 | CB | TRP | 251 | 118.284 | 53.889 | 40.657 | 1.00 | 51.89 |
| | 2277 | CG | TRP | 251 | 117.358 | 53.872 | 41.836 | 1.00 | 58.17 |
| 50 | 2278 | CD1 | TRP | 251 | 117.596 | 54.402 | 43.071 | 1.00 | 60.91 |
| | 2279 | CD2 | TRP | 251 | 116.069 | 53.246 | 41.908 | 1.00 | 60.72 |
| | 2280 | NE1 | TRP | 251 | 116.541 | 54.136 | 43.912 | 1.00 | 64.22 |

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|----|-------|-----|-----|-----|---------|--------|--------|------|-------|
| | 2281 | CE2 | TRP | 251 | 115.589 | 53.429 | 43.225 | 1.00 | 60.87 |
| | 2282 | CE3 | TRP | 251 | 115.274 | 52.546 | 40.989 | 1.00 | 56.90 |
| | 2283 | CZ2 | TRP | 251 | 114.351 | 52.934 | 43.648 | 1.00 | 58.08 |
| | 2284 | CZ3 | TRP | 251 | 114.042 | 52.054 | 41.410 | 1.00 | 53.15 |
| 5 | 2285 | CH2 | TRP | 251 | 113.594 | 52.252 | 42.729 | 1.00 | 53.35 |
| | 2286 | H | TRP | 251 | 119.485 | 54.076 | 38.442 | 1.00 | 25.00 |
| | 2287 | HE1 | TRP | 251 | 116.481 | 54.409 | 44.851 | 1.00 | 25.00 |
| | 2288 | N | LYS | 252 | 119.049 | 56.875 | 40.167 | 1.00 | 64.71 |
| | 2289 | CA | LYS | 252 | 119.191 | 58.241 | 40.661 | 1.00 | 68.07 |
| 10 | 2290 | C | LYS | 252 | 118.440 | 59.227 | 39.779 | 1.00 | 65.20 |
| | 2291 | O | LYS | 252 | 117.831 | 60.169 | 40.283 | 1.00 | 65.28 |
| | 2292 | CB | LYS | 252 | 120.668 | 58.621 | 40.755 | 1.00 | 75.64 |
| | 2293 | CG | LYS | 252 | 121.400 | 57.815 | 41.803 | 1.00 | 85.57 |
| | 2294 | CD | LYS | 252 | 122.890 | 57.818 | 41.588 | 1.00 | 92.92 |
| 15 | 2295 | CE | LYS | 252 | 123.526 | 56.776 | 42.486 | 1.00 | 95.43 |
| | 2296 | NZ | LYS | 252 | 124.902 | 56.526 | 42.101 | 1.00 | 94.64 |
| | 2297 | H | LYS | 252 | 119.849 | 56.379 | 39.887 | 1.00 | 25.00 |
| | 22998 | 1HZ | LYS | 252 | 125.056 | 56.256 | 41.101 | 1.00 | 25.00 |
| | 2299 | 2HZ | LYS | 252 | 125.376 | 57.437 | 42.219 | 1.00 | 25.00 |
| 20 | 2300 | 3HZ | LYS | 252 | 125.417 | 55.867 | 42.716 | 1.00 | 25.00 |
| | 2301 | N | ASP | 253 | 118.453 | 58.983 | 38.469 | 1.00 | 63.40 |
| | 2302 | CA | ASP | 253 | 117.762 | 59.846 | 37.515 | 1.00 | 63.30 |
| | 2303 | C | ASP | 253 | 116.265 | 59.872 | 37.796 | 1.00 | 63.95 |
| | 2304 | O | ASP | 253 | 115.635 | 60.925 | 37.729 | 1.00 | 68.15 |
| 25 | 2305 | CB | ASP | 253 | 118.003 | 59.376 | 36.077 | 1.00 | 68.18 |
| | 2306 | CG | ASP | 253 | 119.467 | 59.453 | 35.664 | 1.00 | 76.46 |
| | 2307 | OD1 | ASP | 253 | 120.293 | 60.015 | 36.419 | 1.00 | 78.84 |
| | 2308 | OD2 | ASP | 253 | 119.793 | 58.943 | 34.570 | 1.00 | 79.35 |
| | 2309 | H | ASP | 253 | 118.948 | 58.203 | 38.137 | 1.00 | 25.00 |
| 30 | 2310 | N | LEU | 254 | 115.697 | 58.710 | 38.105 | 1.00 | 66.44 |
| | 2311 | CA | LEU | 254 | 114.271 | 58.611 | 38.409 | 1.00 | 65.57 |
| | 2312 | C | LEU | 254 | 113.947 | 59.482 | 39.616 | 1.00 | 67.65 |
| | 2313 | O | LEU | 254 | 112.815 | 59.931 | 39.784 | 1.00 | 68.72 |
| | 2314 | CB | LEU | 254 | 113.885 | 57.162 | 38.698 | 1.00 | 61.14 |
| 35 | 2315 | CG | LEU | 254 | 114.124 | 56.166 | 37.564 | 1.00 | 57.75 |
| | 2316 | CD1 | LEU | 254 | 113.718 | 54.785 | 38.021 | 1.00 | 58.43 |
| | 2317 | CD2 | LEU | 254 | 113.343 | 56.571 | 36.328 | 1.00 | 55.32 |
| | 2318 | H | LEU | 254 | 116.252 | 57.902 | 38.125 | 1.00 | 25.00 |
| | 2319 | N | ASP | 255 | 114.947 | 59.661 | 40.475 | 1.00 | 73.64 |
| 40 | 2320 | CA | ASP | 255 | 114.842 | 60.490 | 41.670 | 1.00 | 78.31 |
| | 2321 | C | ASP | 255 | 113.664 | 60.123 | 42.574 | 1.00 | 79.28 |
| | 2322 | O | ASP | 255 | 113.079 | 60.985 | 43.230 | 1.00 | 81.76 |
| | 2323 | CB | ASP | 255 | 114.777 | 61.971 | 41.261 | 1.00 | 83.27 |
| | 2324 | CG | ASP | 255 | 115.238 | 62.915 | 42.364 | 1.00 | 87.17 |
| 45 | 2325 | OD1 | ASP | 255 | 115.719 | 62.443 | 43.420 | 1.00 | 86.98 |
| | 2326 | OD2 | ASP | 255 | 115.121 | 64.144 | 42.165 | 1.00 | 87.49 |
| | 2327 | H | ASP | 255 | 115.805 | 59.226 | 40.294 | 1.00 | 25.00 |
| | 2328 | N | PHE | 256 | 113.357 | 58.834 | 42.659 | 1.00 | 80.00 |
| | 2329 | CA | PHE | 256 | 112.254 | 58.378 | 43.500 | 1.00 | 84.32 |
| 50 | 2330 | C | PHE | 256 | 112.504 | 58.649 | 44.976 | 1.00 | 89.15 |
| | 2331 | O | PHE | 256 | 111.562 | 58.742 | 45.759 | 1.00 | 87.59 |
| | 2332 | CB | PHE | 256 | 111.987 | 56.887 | 43.290 | 1.00 | 81.00 |

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|----|------|-----|-----|-----|---------|--------|---------|------|--------|
| | 2333 | CG | PHE | 256 | 111.352 | 56.566 | 41.972 | 1.00 | 76.86 |
| | 2334 | CD1 | PHE | 256 | 110.671 | 57.544 | 41.251 | 1.00 | 76.59 |
| | 2335 | CD2 | PHE | 256 | 111.431 | 55.283 | 41.449 | 1.00 | 73.54 |
| | 2336 | CE1 | PHE | 256 | 110.080 | 57.247 | 40.030 | 1.00 | 76.03 |
| 5 | 2337 | CE2 | PHE | 256 | 110.844 | 54.976 | 40.229 | 1.00 | 71.61 |
| | 2338 | CZ | PHE | 256 | 110.167 | 55.958 | 39.518 | 1.00 | 74.95 |
| | 2339 | H | PHE | 256 | 113.874 | 58.189 | 42.139 | 1.00 | 25.00 |
| | 2340 | N | VAL | 257 | 113.774 | 58.796 | 45.344 | 1.00 | 97.79 |
| | 2341 | CA | VAL | 257 | 114.160 | 59.053 | 46.730 | 1.00 | 104.36 |
| 10 | 2342 | C | VAL | 257 | 113.428 | 60.269 | 47.303 | 1.00 | 105.53 |
| | 2343 | O | VAL | 257 | 112.952 | 60.239 | 48.439 | 1.00 | 106.91 |
| | 2344 | CB | VAL | 257 | 115.692 | 59.270 | 46.854 | 1.00 | 107.20 |
| | 2345 | CG1 | VAL | 257 | 116.092 | 59.432 | 48.316 | 1.00 | 107.16 |
| | 2346 | CG2 | VAL | 257 | 116.445 | 58.101 | 46.220 | 1.00 | 106.33 |
| 15 | 2347 | H | VAL | 257 | 114.464 | 58.732 | 44.658 | 1.00 | 25.00 |
| | 2348 | N | THR | 258 | 113.332 | 61.329 | 46.5506 | 1.00 | 105.84 |
| | 2349 | CA | THR | 258 | 112.660 | 62.550 | 46.935 | 1.00 | 104.41 |
| | 2350 | C | THR | 258 | 111.183 | 62.608 | 46.531 | 1.00 | 104.31 |
| | 2351 | O | THR | 258 | 110.339 | 63.047 | 47.314 | 1.00 | 104.07 |
| 20 | 2352 | CB | THR | 258 | 113.392 | 63.805 | 46.408 | 1.00 | 104.30 |
| | 2353 | OG1 | THR | 258 | 113.620 | 63.674 | 45.000 | 1.00 | 104.41 |
| | 2354 | CG2 | THR | 258 | 114.729 | 63.982 | 47.117 | 1.00 | 105.42 |
| | 2355 | H | THR | 258 | 113.711 | 61.308 | 45.603 | 1.00 | 25.00 |
| | 2356 | HG1 | THR | 258 | 114.068 | 64.458 | 44.669 | 1.00 | 25.00 |
| 25 | 2357 | N | THR | 259 | 110.872 | 62.161 | 45.317 | 1.00 | 103.41 |
| | 2358 | CA | THR | 259 | 109.497 | 62.182 | 44.825 | 1.00 | 100.89 |
| | 2359 | C | THR | 259 | 108.599 | 61.133 | 45.482 | 1.00 | 101.97 |
| | 2360 | O | THR | 259 | 107.414 | 61.375 | 45.707 | 1.00 | 103.53 |
| | 2361 | CB | THR | 259 | 109.445 | 62.022 | 43.289 | 1.00 | 97.37 |
| 30 | 2362 | OG1 | THR | 259 | 110.219 | 60.883 | 42.894 | 1.00 | 95.69 |
| | 2363 | CG2 | THR | 259 | 109.988 | 63.267 | 42.602 | 1.00 | 95.50 |
| | 2364 | H | THR | 259 | 111.579 | 61.811 | 44.728 | 1.00 | 25.00 |
| | 2365 | HG1 | THR | 259 | 109.870 | 60.086 | 43.290 | 1.00 | 25.00 |
| | 2366 | N | LEU | 260 | 109.164 | 59.969 | 45.783 | 1.00 | 102.18 |
| 35 | 2367 | CA | LEU | 260 | 108.415 | 58.884 | 46.412 | 1.00 | 103.22 |
| | 2368 | C | LEU | 260 | 109.112 | 58.431 | 47.696 | 1.00 | 106.86 |
| | 2369 | O | LEU | 260 | 109.742 | 57.372 | 47.732 | 1.00 | 107.73 |
| | 2370 | CB | LEU | 260 | 108.282 | 57.700 | 45.445 | 1.00 | 98.81 |
| | 2371 | CG | LEU | 260 | 107.552 | 57.928 | 44.119 | 1.00 | 94.81 |
| 40 | 2372 | CD1 | LEU | 260 | 107.620 | 56.670 | 43.269 | 1.00 | 89.99 |
| | 2373 | CD2 | LEU | 260 | 106.108 | 58.320 | 44.380 | 1.00 | 92.83 |
| | 2374 | H | LEU | 260 | 110.112 | 59.844 | 45.595 | 1.00 | 25.00 |
| | 2375 | N | PRO | 261 | 108.963 | 59.204 | 48.784 | 1.00 | 110.17 |
| | 2376 | CA | PRO | 261 | 109.580 | 58.889 | 50.077 | 1.00 | 112.52 |
| 45 | 2377 | C | PRO | 261 | 108.951 | 57.726 | 50.855 | 1.00 | 114.04 |
| | 2378 | O | PRO | 261 | 108.783 | 57.813 | 52.073 | 1.00 | 117.31 |
| | 2379 | CB | PRO | 261 | 109.441 | 60.207 | 50.836 | 1.00 | 113.40 |
| | 2380 | CG | PRO | 261 | 108.124 | 60.715 | 50.347 | 1.00 | 112.70 |
| | 2381 | CD | PRO | 261 | 108.223 | 60.477 | 48.856 | 1.00 | 111.17 |
| 50 | 2382 | N | TYR | 262 | 108.599 | 56.646 | 50.163 | 1.00 | 113.40 |
| | 2383 | CA | TYR | 262 | 108.012 | 55.479 | 50.822 | 1.00 | 112.08 |
| | 2384 | C | TYR | 262 | 108.608 | 54.178 | 50.284 | 1.00 | 112.01 |

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|----|------|------|-----|-----|---------|--------|--------|-------------|
| | 2385 | O | TYR | 262 | 108.125 | 53.086 | 50.582 | 1.00110.30 |
| | 2386 | CB | TYR | 262 | 106.477 | 55.478 | 50.702 | 1.00109.31 |
| | 2387 | CG | TYR | 262 | 105.931 | 55.286 | 49.303 | 1.00104.93 |
| | 2388 | CD1 | TYR | 262 | 105.777 | 56.369 | 48.440 | 1.00103.18 |
| 5 | 2389 | CD2 | TYR | 262 | 105.555 | 54.021 | 48.846 | 1.00102.84 |
| | 2390 | CE1 | TYR | 262 | 105.262 | 56.201 | 47.159 | 1.00101.09 |
| | 2391 | CE2 | TYR | 262 | 105.040 | 53.842 | 47.565 | 1.00100.35 |
| | 2392 | CZ | TYR | 262 | 104.897 | 54.938 | 46.727 | 1.00100.07 |
| | 2393 | OH | TYR | 262 | 104.386 | 54.781 | 45.459 | 1.00 97.25 |
| 10 | 2394 | H | TYR | 262 | 108.755 | 56.615 | 49.199 | 1.00 25.00 |
| | 2395 | HH | TYR | 262 | 104.276 | 53.862 | 45.236 | 1.00 25.00 |
| | 2396 | N | ALA | 263 | 109.671 | 54.310 | 49.497 | 1.00113.11 |
| | 2397 | CA | ALA | 263 | 110.360 | 53.166 | 48.913 | 1.00114.09 |
| | 2398 | C | ALA | 263 | 111.856 | 53.343 | 49.146 | 1.00114.75 |
| 15 | 2399 | O | ALA | 263 | 112.375 | 54.457 | 49.055 | 1.00115.90 |
| | 2400 | CB | ALA | 263 | 110.064 | 53.077 | 47.428 | 1.00112.96 |
| | 2401 | H | ALA | 263 | 110.034 | 55.202 | 49.305 | 1.00 25.00 |
| | 2402 | N | ARG | 264 | 112.543 | 52.252 | 49.467 | 1.00113.69 |
| | 2403 | CA | ARG | 264 | 113.979 | 52.309 | 49.726 | 1.00114.09 |
| 20 | 2404 | C | ARG | 264 | 114.847 | 51.948 | 48.526 | 1.00109.03 |
| | 2405 | O | ARG | 264 | 114.394 | 51.280 | 47.594 | 1.00109.80 |
| | 2406 | CB | ARG | 264 | 114.355 | 51.448 | 50.945 | 1.00116.51 |
| | 2407 | CG | ARG | 264 | 113.434 | 50.258 | 51.235 | 1.00118.71 |
| | 2408 | CD | ARG | 264 | 113.486 | 49.190 | 50.151 | 1.00120.73 |
| 25 | 2409 | NE | ARG | 264 | 112.543 | 48.105 | 50.418 | 1.00118.02 |
| | 2410 | CZ | ARG | 264 | 111.607 | 47.696 | 49.565 | 1.00115.79 |
| | 2411 | NH1 | ARG | 264 | 111.479 | 48.277 | 48.380 | 1.00114..07 |
| | 2412 | NH2 | ARG | 264 | 110.788 | 46.709 | 49.904 | 1.00113.33 |
| | 2413 | H | ARG | 264 | 112.079 | 51.393 | 49.495 | 1.00 25.00 |
| 30 | 2414 | HE | ARG | 264 | 112.602 | 47.651 | 51.284 | 1.00 25.00 |
| | 2415 | 1HH1 | ARG | 264 | 112.083 | 49.029 | 48.120 | 1.00 25.00 |
| | 2416 | 2HH1 | ARG | 264 | 110.766 | 47.967 | 47.751 | 1.00 25.00 |
| | 2417 | 1HH2 | ARG | 264 | 110.868 | 46.283 | 50.807 | 1.00 25.00 |
| | 2418 | 2HH2 | ARG | 264 | 110.074 | 46.408 | 49.273 | 1.00 25.00 |
| 35 | 2419 | N | ASP | 265 | 116.089 | 52.421 | 48.550 | 1.00103.18 |
| | 2420 | CA | ASP | 265 | 117.045 | 52.152 | 47.485 | 1.00 97.60 |
| | 2421 | C | ASP | 265 | 117.480 | 50.688 | 47.579 | 1.00 92.70 |
| | 2422 | O | ASP | 265 | 118.533 | 50.371 | 48.138 | 1.00 96.57 |
| | 2423 | CB | ASP | 265 | 118.255 | 53.086 | 47.619 | 1.00100.16 |
| 40 | 2424 | CG | ASP | 265 | 119.317 | 52.826 | 46.565 | 1.00106.00 |
| | 2425 | OD1 | ASP | 265 | 118.992 | 52.887 | 45.363 | 1.00107.25 |
| | 2426 | OD2 | ASP | 265 | 120.479 | 52.556 | 46.940 | 1.00109.23 |
| | 2427 | H | ASP | 265 | 116.373 | 52.965 | 49.310 | 1.00 25.00 |
| | 2428 | N | ARG | 266 | 116.654 | 49.799 | 47.041 | 1.00 82.19 |
| 45 | 2429 | CA | ARG | 266 | 116.942 | 48.372 | 47.073 | 1.00 73.27 |
| | 2430 | C | ARG | 266 | 117.613 | 47.910 | 45.775 | 1.00 63.23 |
| | 2431 | O | ARG | 266 | 117.711 | 46.712 | 45.511 | 1.00 66.31 |
| | 2432 | CB | ARG | 266 | 115.646 | 47.585 | 47.320 | 1.00 77.54 |
| | 2433 | CG | ARG | 266 | 115.801 | 46.402 | 48.274 | 1.00 83.80 |
| 50 | 2434 | CD | ARG | 266 | 114.480 | 45.672 | 48.520 | 1.00 86.40 |
| | 2435 | NE | ARG | 266 | 114.015 | 44.911 | 47.358 | 1.00 87.97 |
| | 2436 | CZ | ARG | 266 | 114.383 | 43.661 | 47.077 | 1.00 87.83 |

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|----|------|------|-----|------|---------|--------|--------|------|-------|
| | 2437 | NH1 | ARG | 266 | 115.229 | 43.014 | 47.869 | 1.00 | 86.43 |
| | 2438 | NH2 | ARG | 266 | 113.895 | 43.049 | 46.005 | 1.00 | 80.67 |
| | 2439 | H | ARG | 266 | 115.816 | 50.112 | 46.631 | 1.00 | 25.00 |
| | 2440 | HE | ARG | 266 | 113.386 | 45.348 | 46.747 | 1.00 | 25.00 |
| 5 | 2441 | 1HH1 | ARG | 266 | 115.600 | 43.463 | 48.681 | 1.00 | 25.00 |
| | 2442 | 2HH1 | ARG | 266 | 115.502 | 42.079 | 47.647 | 1.00 | 25.00 |
| | 2443 | 1HH2 | ARG | 266 | 113.246 | 43.525 | 45.410 | 1.00 | 25.00 |
| | 2444 | 2HH2 | ARG | 266 | 114.170 | 42.111 | 45.794 | 1.00 | 25.00 |
| | 2445 | N | VAL | 267 | 118.130 | 48.859 | 45.000 | 1.00 | 54.00 |
| 10 | 2446 | CA | VAL | 267 | 118.778 | 48.560 | 43.722 | 1.00 | 46.85 |
| | 2447 | C | VAL | 267 | 119.865 | 47.496 | 43.784 | 1.00 | 44.14 |
| | 2448 | O | VAL | 267 | 119.911 | 46.609 | 42.935 | 1.00 | 45.14 |
| | 2449 | CB | VAL | 267 | 119.361 | 49.827 | 43.076 | 1.00 | 45.45 |
| | 2450 | CG1 | VAL | 267 | 119.991 | 49.499 | 41.733 | 1.00 | 42.99 |
| 15 | 2451 | CG2 | VAL | 267 | 118.273 | 50.848 | 42.892 | 1.00 | 51.05 |
| | 2452 | H | VAL | 267 | 118.072 | 49.785 | 45.299 | 1.00 | 25.00 |
| | 2453 | N | VAL | 268 | 120.738 | 47.576 | 44.781 | 1.00 | 40.56 |
| | 2454 | CA | VAL | 268 | 121.813 | 46.597 | 44.910 | 1.00 | 38.21 |
| | 2455 | C | VAL | 268 | 121.242 | 45.185 | 45.125 | 1.00 | 35.40 |
| 20 | 2456 | O | VAL | 268 | 121.708 | 44.220 | 44.513 | 1.00 | 29.56 |
| | 2457 | CB | VAL | 268 | 122.785 | 46.976 | 46.046 | 1.00 | 40.34 |
| | 2458 | CG1 | VAL | 268 | 123.983 | 46.055 | 46.040 | 1.00 | 41.41 |
| | 2459 | CG2 | VAL | 268 | 123.239 | 48.414 | 45.880 | 1.00 | 43.02 |
| | 2460 | H | VAL | 268 | 120.663 | 48.303 | 45.428 | 1.00 | 25.00 |
| 25 | 2461 | N | GLU | 269 | 120.202 | 45.081 | 45.952 | 1.00 | 33.49 |
| | 2462 | CA | GLU | 2669 | 119.553 | 43.796 | 46.220 | 1.00 | 31.75 |
| | 2463 | C | GLU | 269 | 118.910 | 43.278 | 44.936 | 1.00 | 31.29 |
| | 2464 | O | GLU | 269 | 119.023 | 42.095 | 44.607 | 1.00 | 34.74 |
| | 2465 | CB | GLU | 269 | 118.477 | 43.940 | 47.300 | 1.00 | 30.42 |
| 30 | 2466 | CG | GLU | 269 | 118.998 | 44.124 | 48.719 | 1.00 | 41.96 |
| | 2467 | CD | GLU | 269 | 119.777 | 45.418 | 48.921 | 1.00 | 53.70 |
| | 2468 | OE1 | GLU | 269 | 119.387 | 46.465 | 48.356 | 1.00 | 52.14 |
| | 2469 | OE2 | GLU | 269 | 120.785 | 45.385 | 49.658 | 1.00 | 60.44 |
| | 2470 | H | GLU | 269 | 119.849 | 45.888 | 46.369 | 1.00 | 25.00 |
| 35 | 2471 | N | CYS | 270 | 118.258 | 44.179 | 44.204 | 1.00 | 25.87 |
| | 2472 | CA | CYS | 270 | 117.603 | 43.829 | 42.948 | 1.00 | 31.04 |
| | 2473 | C | CYS | 270 | 118.628 | 43.330 | 41.944 | 1.00 | 31.66 |
| | 2474 | O | CYS | 270 | 118.352 | 42.406 | 41.170 | 1.00 | 34.14 |
| | 2475 | CB | CYS | 270 | 116.841 | 45.029 | 42.380 | 1.00 | 31.00 |
| 40 | 2476 | SG | CYS | 270 | 115.468 | 45.566 | 43.429 | 1.00 | 41.23 |
| | 2477 | H | CYS | 270 | 118.204 | 45.102 | 44.523 | 1.00 | 25.00 |
| | 2478 | N | TYR | 271 | 119.817 | 43.927 | 41.968 | 1.00 | 30.55 |
| | 2479 | CA | TYR | 271 | 120.875 | 43.506 | 41.065 | 1.00 | 29.41 |
| | 2480 | C | TYR | 271 | 121.365 | 42.109 | 41.459 | 1.00 | 29.51 |
| 45 | 2481 | O | TYR | 271 | 121.662 | 41.284 | 40.592 | 1.00 | 30.16 |
| | 2482 | CB | TYR | 271 | 122.048 | 44.496 | 41.048 | 1.00 | 27.85 |
| | 2483 | CG | TYR | 271 | 123.125 | 44.061 | 40.077 | 1.00 | 27.35 |
| | 2484 | CD1 | TYR | 271 | 123.006 | 44.327 | 38.714 | 1.00 | 25.72 |
| | 2485 | CD2 | TYR | 271 | 124.198 | 43.279 | 40.502 | 1.00 | 20.62 |
| 50 | 2486 | CE1 | TYR | 271 | 123.923 | 43.813 | 37.798 | 1.00 | 22.98 |
| | 2487 | CE2 | TYR | 271 | 125.116 | 42.762 | 39.593 | 1.00 | 27.42 |
| | 2488 | CZ | TYR | 271 | 124.970 | 43.030 | 38.245 | 1.00 | 21.79 |

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|----|------|------|-----|-----|----------|--------|--------|------|-------|
| | 2489 | OH | TYR | 271 | 125.859 | 42.497 | 37.343 | 1.00 | 23.43 |
| | 2490 | H | TYR | 271 | 119.985 | 44.662 | 42.594 | 1.00 | 25.00 |
| | 2491 | HH | TYR | 271 | 126.485 | 41.987 | 37.843 | 1.00 | 25.00 |
| | 2492 | N | PHE | 272 | 121.453 | 41.845 | 42.760 | 1.00 | 26.47 |
| 5 | 2493 | CA | PHE | 272 | 121.892 | 40.535 | 43.220 | 1.00 | 28.71 |
| | 2494 | C | PHE | 272 | 120.957 | 39.486 | 42.633 | 1.00 | 31.32 |
| | 2495 | O | PHE | 272 | 121.408 | 38.470 | 42.102 | 1.00 | 31.50 |
| | 2496 | CB | PHE | 272 | 121.881 | 40.442 | 44.747 | 1.00 | 32.54 |
| | 2497 | CG | PHE | 272 | 122.165 | 39.058 | 45.264 | 1.00 | 34.15 |
| 10 | 2498 | CD1 | PHE | 272 | 123.471 | 38.577 | 45.323 | 1.00 | 32.37 |
| | 2499 | CD2 | PHE | 272 | 121.120 | 38.211 | 45.638 | 1.00 | 34.09 |
| | 2500 | CE11 | PHE | 272 | 123.732 | 37.271 | 45.739 | 1.00 | 35.66 |
| | 2501 | CE2 | PHE | 272 | 121.369 | 36.902 | 46.055 | 1.00 | 34.18 |
| | 2502 | CZ | PHE | 272 | 122.679 | 36.431 | 46.105 | 1.00 | 36.58 |
| 15 | 2503 | H | PHE | 272 | 121.228 | 42.541 | 43.413 | 1.00 | 25.00 |
| | 2504 | N | TRP | 273 | 119.656 | 39.744 | 42.712 | 1.00 | 29.73 |
| | 2505 | CA | TRP | 273 | 118.670 | 38.817 | 42.167 | 1.00 | 30.60 |
| | 2506 | C | TRP | 273 | 118.924 | 38.551 | 40.685 | 1.00 | 30.33 |
| | 2507 | O | TRP | 273 | 118.971 | 37.396 | 40.250 | 1.00 | 32.10 |
| 20 | 2508 | CB | TRP | 273 | 117.255 | 39.357 | 42.365 | 1.00 | 28.17 |
| | 2509 | CG | TRP | 273 | 116.707 | 39.092 | 43.721 | 1.00 | 33.41 |
| | 2510 | CD1 | TRP | 273 | 117.241 | 39.478 | 44.915 | 1.00 | 37.71 |
| | 2511 | CD2 | TRP | 273 | 115.506 | 38.381 | 44.029 | 1.00 | 41.82 |
| | 2512 | NE1 | TRP | 273 | 116.445 | 39.053 | 45.950 | 1.00 | 39.11 |
| 25 | 2513 | CE2 | TRP | 273 | 115.372 | 38.378 | 45.435 | 1.00 | 43.90 |
| | 2514 | CE3 | TRP | 273 | 114.528 | 37.747 | 43.253 | 1.00 | 47.13 |
| | 2515 | CZ2 | TRP | 273 | 114.296 | 37.764 | 46.083 | 1.00 | 49.35 |
| | 2516 | CZ3 | TRP | 273 | 113.458 | 37.136 | 43.898 | 1.00 | 53.38 |
| | 2517 | CH2 | TRP | 273 | 113.352 | 37.150 | 45.300 | 1.00 | 53.17 |
| 30 | 2518 | H | TRP | 273 | 119.359 | 40.569 | 43.153 | 1.00 | 25.00 |
| | 2519 | HE1 | TRP | 273 | 116.622 | 39.201 | 46.903 | 1.00 | 25.00 |
| | 2520 | N | ALA | 274 | 119.117 | 39.617 | 39.915 | 1.00 | 26.20 |
| | 2521 | CA | ALA | 274 | 119.371 | 39.472 | 38.489 | 1.00 | 25.12 |
| | 2522 | C | ALA | 274 | 120.638 | 38.657 | 38.263 | 1.00 | 27.03 |
| 35 | 2523 | O | ALA | 274 | 120.686 | 37.816 | 37.366 | 1.00 | 29.08 |
| | 2524 | CB | ALA | 274 | 119.491 | 40.832 | 37.831 | 1.00 | 22.68 |
| | 2525 | H | ALA | 274 | 119.0884 | 40.514 | 40.313 | 1.00 | 25.00 |
| | 2526 | N | LEU | 275 | 121.646 | 38.886 | 39.104 | 1.00 | 26.74 |
| | 2527 | CA | LEU | 275 | 122.922 | 38.175 | 39.011 | 1.00 | 23.65 |
| 40 | 2528 | C | LEU | 275 | 122.727 | 36.689 | 39.329 | 1.00 | 20.19 |
| | 2529 | O | LEU | 275 | 123.432 | 35.825 | 38.798 | 1.00 | 18.69 |
| | 2530 | CB | LEU | 275 | 123.945 | 38.802 | 39.963 | 1.00 | 22.77 |
| | 2531 | CG | LEU | 275 | 125.377 | 38.280 | 39.867 | 1.00 | 22.23 |
| | 2532 | CD1 | LEU | 275 | 125.859 | 38.352 | 38.427 | 1.00 | 20.45 |
| 45 | 2533 | CD2 | LEU | 275 | 126.274 | 39.097 | 40.779 | 1.00 | 24.10 |
| | 2534 | H | LEU | 275 | 121.532 | 39.552 | 39.808 | 1.00 | 25.00 |
| | 2535 | N | GLY | 276 | 121.765 | 36.406 | 40.204 | 1.00 | 19.17 |
| | 2536 | CA | GLY | 276 | 121.453 | 35.035 | 40.561 | 1.00 | 19.61 |
| | 2537 | C | GLY | 276 | 120.811 | 34.299 | 39.392 | 1.00 | 25.48 |
| 50 | 2538 | O | GLY | 276 | 121.060 | 33.108 | 39.199 | 1.00 | 28.59 |
| | 2539 | H | GLY | 276 | 121.266 | 37.137 | 40.623 | 1.00 | 25.00 |
| | 2540 | N | VAL | 277 | 120.000 | 35.006 | 38.603 | 1.00 | 20.84 |

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|----|------|-----|-----|-----|---------|--------|---------|------|-------|
| | 2541 | CA | VAL | 277 | 119.323 | 34.415 | 37.440 | 1.00 | 19.19 |
| | 2542 | C | VAL | 277 | 120.304 | 34.028 | 36.319 | 1.00 | 19.17 |
| | 2543 | O | VAL | 277 | 120.086 | 33.048 | 35.606 | 1.00 | 21.35 |
| | 2544 | CB | VAL | 277 | 118.201 | 35.355 | 36.904 | 1.00 | 21.19 |
| 5 | 2545 | CG1 | VAL | 277 | 117.560 | 34.777 | 35.650 | 1.00 | 15.33 |
| | 2546 | CG2 | VAL | 277 | 117.138 | 35.550 | 37.976 | 1.00 | 11.13 |
| | 2547 | H | VAL | 277 | 119.858 | 35.954 | 38.810 | 1.00 | 25.00 |
| | 2548 | N | TYR | 278 | 121.345 | 34.834 | 36.137 | 1.00 | 21.16 |
| | 2549 | CA | TYR | 278 | 122.401 | 34.587 | 35.150 | 1.00 | 24.77 |
| 10 | 2550 | C | TYR | 278 | 123.583 | 35.532 | 35.351 | 1.00 | 29.35 |
| | 2551 | O | TYR | 278 | 123.405 | 36.738 | 35.531 | 1.00 | 27.69 |
| | 2552 | CB | TYR | 278 | 121.910 | 34.611 | 33.687 | 1.00 | 25.96 |
| | 2553 | CG | TYR | 278 | 120.741 | 35.517 | 33.341 | 1.00 | 26.89 |
| | 2554 | CD1 | TYR | 278 | 120.580 | 36.768 | 33.937 | 1.00 | 25.88 |
| 15 | 2555 | CD2 | TYR | 278 | 119.800 | 35.116 | 32.388 | 1.00 | 27.14 |
| | 2556 | CE1 | TYR | 278 | 119.508 | 37.595 | 33.594 | 1.00 | 29.19 |
| | 2557 | CE2 | TYR | 278 | 118.729 | 35.934 | 32.037 | 1.00 | 31.49 |
| | 2558 | CZ | TYR | 278 | 118.587 | 37.171 | 32.643 | 1.00 | 31.78 |
| | 2559 | OH | TYR | 278 | 117.522 | 37.976 | 32.301 | 1.00 | 31.66 |
| 20 | 2560 | H | TYR | 278 | 121.419 | 35.652 | 36.684 | 1.00 | 25.00 |
| | 2561 | HH | TYR | 278 | 117.022 | 37.548 | 31.600 | 1.00 | 25.00 |
| | 2562 | N | PHE | 279 | 124.789 | 34.968 | 35.332 | 1.00 | 31.85 |
| | 2563 | CA | PHE | 279 | 126.017 | 35.732 | 35.549 | 1.00 | 28.28 |
| | 2564 | C | PHE | 279 | 126.910 | 35.844 | 34.318 | 1.00 | 28.86 |
| 25 | 2565 | O | PHE | 279 | 127.855 | 36.636 | 34.310 | 1.00 | 28.24 |
| | 2566 | CB | PHE | 279 | 126.829 | 35.087 | 36.678 | 1.00 | 24.38 |
| | 2567 | CG | PHE | 279 | 127.334 | 33.707 | 36.344 | 1.00 | 23.04 |
| | 2568 | CD1 | PHE | 279 | 128.563 | 33.535 | 35.706 | 1.00 | 16.44 |
| | 2569 | CD2 | PHE | 279 | 126.557 | 32.582 | 36.616 | 1.00 | 22.61 |
| 30 | 2570 | CE1 | PHE | 279 | 129.005 | 32.265 | 35.339 | 1.00 | 22.82 |
| | 2571 | CE2 | PHE | 279 | 126.989 | 31.309 | 36.254 | 1.00 | 22.81 |
| | 2572 | CZ | PHE | 279 | 128.214 | 31.149 | 35.613 | 1.00 | 20.63 |
| | 2573 | H | PHE | 279 | 124.845 | 34.006 | 35.181 | 1.00 | 25.00 |
| | 2574 | N | GLU | 280 | 126.653 | 35.010 | 33.315 | 1.00 | 25.83 |
| 35 | 2575 | CA | GLU | 280 | 127.450 | 34.995 | 32.093 | 1.00 | 25.96 |
| | 2576 | C | GLU | 280 | 127.464 | 36.347 | 31.384 | 1.00 | 32.09 |
| | 2577 | O | GLU | 280 | 126.461 | 37.067 | 31.378 | 1.00 | 33.29 |
| | 2578 | CB | GLU | 280 | 126.947 | 33.909 | 31.140 | 1.00 | 29.64 |
| | 2579 | CG | GLU | 280 | 127.116 | 32.479 | 31.652 | 1.00 | 31.98 |
| 40 | 2580 | CD | GLU | 280 | 125.873 | 31.921 | 32.338 | 1.00 | 41.40 |
| | 2581 | OE1 | GLU | 280 | 125.089 | 32.696 | 32.938 | 1.00 | 33.42 |
| | 2582 | OE2 | GLU | 280 | 125.681 | 30.688 | 32.273 | 1.00 | 43.76 |
| | 2583 | H | GLU | 280 | 125.894 | 34.421 | 33.402 | 1.00 | 25.00 |
| | 2584 | N | PRO | 281 | 128.593 | 36.687 | 30.735 | 1.00 | 34.75 |
| 45 | 2585 | CA | PRO | 281 | 128.736 | 37.961 | 30.018 | 1.00 | 32.48 |
| | 2586 | C | PRO | 281 | 127.718 | 38.182 | 28.899 | 1.00 | 30.11 |
| | 2587 | O | PRO | 281 | 127.273 | 39.309 | 28.675 | 1.00 | 33.55 |
| | 2588 | CB | PRO | 281 | 130.177 | 37.901 | 229.492 | 1.00 | 33.45 |
| | 2589 | CG | PRO | 281 | 130.447 | 36.426 | 29.366 | 1.00 | 34.83 |
| 50 | 2590 | CD | PRO | 281 | 129.824 | 35.882 | 30.625 | 1.00 | 32.94 |
| | 2591 | N | GLN | 282 | 127.319 | 37.106 | 28.226 | 1.00 | 30.38 |
| | 2592 | CA | GLN | 282 | 126.350 | 37.195 | 27.134 | 1.00 | 31.74 |

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|----|------|------|------|-----|---------|--------|--------|------|-------|
| | 2593 | C | GLN | 282 | 124.980 | 37.704 | 27.600 | 1.00 | 33.53 |
| | 2594 | O | GLN | 282 | 124.194 | 38.202 | 26.792 | 1.00 | 34.52 |
| | 2595 | CB | GLN | 282 | 126.183 | 35.829 | 26.462 | 1.00 | 35.52 |
| | 2596 | CG | GLN | 282 | 125.442 | 34.819 | 27.323 | 1.00 | 47.53 |
| 5 | 2597 | CD | GLN | 282 | 125.543 | 33.400 | 26.807 | 1.00 | 54.68 |
| | 2598 | OE1 | GLN | 282 | 126.378 | 32.624 | 27.273 | 1.00 | 58.66 |
| | 2599 | NE2 | GLN | 282 | 124.675 | 33.040 | 25.866 | 1.00 | 55.48 |
| | 2600 | H | GLN | 282 | 127.685 | 36.233 | 28.468 | 1.00 | 25.00 |
| | 2601 | 1HE2 | GLLN | 282 | 124.740 | 32.122 | 25.538 | 1.00 | 25.00 |
| 10 | 2602 | 2HE2 | GLN | 282 | 124.018 | 33.690 | 25.551 | 1.00 | 25.00 |
| | 2603 | N | TYR | 283 | 124.698 | 37.577 | 28.896 | 1.00 | 27.81 |
| | 2604 | CA | TYR | 283 | 123.417 | 38.015 | 29.447 | 1.00 | 26.64 |
| | 2605 | C | TYR | 283 | 123.470 | 39.392 | 30.099 | 1.00 | 29.80 |
| | 2606 | O | TYR | 283 | 122.615 | 39.732 | 30.922 | 1.00 | 29.85 |
| 15 | 2607 | CB | TYR | 283 | 122.885 | 36.982 | 30.444 | 1.00 | 24.82 |
| | 2608 | CG | TYR | 283 | 122.670 | 35.614 | 29.840 | 1.00 | 26.77 |
| | 2609 | CD1 | TYR | 283 | 121.786 | 35.432 | 28.775 | 1.00 | 28.94 |
| | 2610 | CD2 | TYR | 283 | 123.373 | 34.506 | 30.313 | 1.00 | 26.51 |
| | 2611 | CE1 | TYR | 283 | 121.610 | 34.174 | 28.192 | 1.00 | 32.76 |
| 20 | 2612 | CE2 | TYR | 283 | 123.205 | 33.247 | 29.740 | 1.00 | 28.52 |
| | 2613 | CZ | TYR | 283 | 122.324 | 33.086 | 28.680 | 1.00 | 30.97 |
| | 2614 | OH | TYR | 283 | 122.164 | 31.845 | 28.104 | 1.00 | 25.13 |
| | 2615 | H | TYR | 283 | 125.361 | 37.198 | 29.509 | 1.00 | 25.00 |
| | 2616 | HH | TYR | 283 | 122.723 | 31.208 | 28.556 | 1.00 | 25.00 |
| 25 | 2617 | N | SER | 284 | 124.449 | 40.196 | 29.697 | 1.00 | 30.66 |
| | 2618 | CA | SER | 284 | 124.620 | 41.539 | 30.239 | 1.00 | 33.15 |
| | 2619 | C | SER | 284 | 123.375 | 42.412 | 30.040 | 1.00 | 32.37 |
| | 2620 | O | SER | 284 | 122.858 | 42.999 | 30.999 | 1.00 | 32.25 |
| | 2621 | CB | SER | 284 | 125.848 | 42.201 | 29.609 | 1.00 | 32.60 |
| 30 | 2622 | OG | SER | 284 | 126.037 | 43.511 | 30.110 | 1.00 | 38.65 |
| | 2623 | H | SER | 284 | 125.090 | 39.876 | 29.027 | 1.00 | 25.00 |
| | 2624 | HG | SER | 284 | 126.140 | 43.520 | 31.058 | 1.00 | 25.00 |
| | 2625 | N | GLN | 285 | 122.882 | 42.477 | 28.805 | 1.00 | 35.28 |
| | 2626 | CA | GLN | 285 | 121.693 | 43.273 | 28.505 | 1.00 | 36.59 |
| 35 | 2627 | C | GLN | 285 | 120.489 | 42.735 | 29.284 | 1.00 | 33.06 |
| | 2628 | O | GLN | 285 | 119.713 | 43.504 | 29.856 | 1.00 | 33.43 |
| | 2629 | CB | GLN | 285 | 121.399 | 43.255 | 27.002 | 1.00 | 36.57 |
| | 2630 | CG | GLN | 285 | 120.138 | 44.020 | 26.611 | 1.00 | 48.54 |
| | 2631 | CD | GLN | 285 | 119.829 | 43.943 | 25.123 | 1.00 | 54.77 |
| 40 | 2632 | OE1 | GLN | 285 | 120.079 | 42.927 | 24.470 | 1.00 | 55.77 |
| | 2633 | NE2 | GLN | 285 | 119.280 | 45.024 | 24.581 | 1.00 | 56.33 |
| | 2634 | H | GLN | 285 | 123.323 | 41.984 | 28.086 | 1.00 | 25.00 |
| | 2635 | 1HE2 | GLN | 285 | 119.084 | 44.982 | 23.621 | 1.00 | 25.00 |
| | 2636 | 2HE2 | GLN | 285 | 119.099 | 45.802 | 25.141 | 1.00 | 25.00 |
| 45 | 2637 | N | ALA | 286 | 120.364 | 41.410 | 29.324 | 1.00 | 32.38 |
| | 2638 | CA | ALA | 286 | 119.272 | 40.750 | 30.032 | 1.00 | 28.79 |
| | 2639 | C | ALA | 286 | 119.254 | 41.117 | 31.512 | 1.00 | 26.70 |
| | 2640 | O | ALA | 286 | 118.200 | 41.438 | 32.060 | 1.00 | 31.71 |
| | 2641 | CB | ALA | 286 | 119.370 | 39.244 | 29.859 | 1.00 | 30.35 |
| 50 | 2642 | H | ALA | 286 | 121.023 | 40.859 | 28.861 | 1.00 | 25.00 |
| | 2643 | N | ARG | 287 | 120.422 | 41.097 | 32.152 | 1.00 | 26.48 |
| | 2644 | CA | ARG | 287 | 120.517 | 41.442 | 33.568 | 1.00 | 27.31 |

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|----|------|------|-----|-----|---------|--------|---------|------|-------|
| | 2645 | C | ARG | 287 | 120.056 | 42.870 | 33.826 | 1.00 | 27.08 |
| | 2646 | O | ARG | 287 | 119.290 | 43.118 | 34.760 | 1.00 | 28.78 |
| | 2647 | CB | ARG | 287 | 121.946 | 41.266 | 34.096 | 1.00 | 28.17 |
| | 2648 | CG | ARG | 287 | 122.240 | 39.891 | 34.652 | 1.00 | 25.50 |
| 5 | 2649 | CD | ARG | 287 | 123.566 | 39.859 | 35.396 | 1.00 | 24.46 |
| | 2650 | NE | ARG | 287 | 124.703 | 40.191 | 34.535 | 1.00 | 20.40 |
| | 2651 | CZ | ARG | 287 | 125.252 | 39.373 | 33.641 | 1.00 | 23.12 |
| | 2652 | NH1 | ARG | 287 | 124.781 | 38.146 | 33.473 | 1.00 | 23.32 |
| | 2653 | NH2 | ARG | 287 | 126.268 | 39.793 | 32.897 | 1.00 | 22.53 |
| 10 | 2654 | H | ARG | 287 | 121.232 | 40.840 | 31.670 | 1.00 | 25.00 |
| | 2655 | HE | ARG | 287 | 125.093 | 41.059 | 34.627 | 1.00 | 25.00 |
| | 2656 | 1HH1 | ARG | 287 | 124.002 | 37.833 | 34.014 | 1.00 | 25.00 |
| | 2657 | 2HH1 | ARG | 287 | 125.192 | 37.542 | 32.796 | 1.00 | 25.00 |
| | 2658 | 1HH2 | ARG | 287 | 126.623 | 40.719 | 33.014 | 1.00 | 25.00 |
| 15 | 2659 | 2HH2 | ARG | 287 | 126.677 | 39.179 | 32.225 | 1.00 | 25.00 |
| | 2660 | N | VAL | 288 | 120.512 | 43.802 | 32.992 | 1.00 | 30.28 |
| | 2661 | CA | VAL | 288 | 120.144 | 45.208 | 33.148 | 1.00 | 29.94 |
| | 2662 | C | VAL | 288 | 118.628 | 45.388 | 33.043 | 1.00 | 28.55 |
| | 2663 | O | VAL | 288 | 118.018 | 46.044 | 33.890 | 1.00 | 35.55 |
| 20 | 2664 | CB | VAL | 288 | 120.874 | 46.106 | 32.120 | 1.00 | 35.29 |
| | 2665 | CG1 | VAL | 288 | 120.536 | 47.572 | 32.363 | 1.00 | 30.30 |
| | 2666 | CG2 | VAL | 288 | 122.378 | 45.896 | 32.221 | 1.00 | 31.86 |
| | 2667 | H | VAL | 288 | 121.107 | 43.535 | 32.256 | 1.00 | 25.00 |
| | 2668 | N | MET | 289 | 118.018 | 44.775 | 32.031 | 1.00 | 27.91 |
| 25 | 2669 | CA | MET | 289 | 116.567 | 44.856 | 31.854 | 1.00 | 27.36 |
| | 2670 | C | MET | 289 | 115.857 | 44.248 | 33.066 | 1.00 | 27.49 |
| | 2671 | O | MET | 289 | 114.938 | 44.845 | 33.627 | 1.00 | 29.43 |
| | 2672 | CB | MET | 289 | 116.136 | 44.129 | 30.572 | 1.00 | 28.18 |
| | 2673 | CG | MET | 289 | 116.578 | 44.819 | 29.282 | 1.00 | 28.82 |
| 30 | 2674 | SD | MET | 289 | 116.207 | 43.882 | 27.770 | 1.00 | 38.33 |
| | 2675 | CE | MET | 289 | 114.526 | 44.384 | 27.438 | 1.00 | 39.91 |
| | 2676 | H | MET | 289 | 118.554 | 44.257 | 31.391 | 1.00 | 25.00 |
| | 2677 | N | LEU | 290 | 116.335 | 43.089 | 33.511 | 1.00 | 25.99 |
| | 2678 | CA | LEU | 290 | 115.743 | 42.408 | 34.654 | 1.00 | 25.33 |
| 35 | 2679 | C | LEU | 290 | 115.805 | 43.222 | 35.949 | 1.00 | 26.44 |
| | 2680 | O | LEU | 290 | 114.815 | 43.289 | 36.687 | 1.00 | 30.04 |
| | 2681 | CB | LEU | 290 | 116.393 | 41.035 | 34.843 | 1.00 | 25.26 |
| | 2682 | CG | LEU | 290 | 115.880 | 40.125 | 35.964 | 1.00 | 25.88 |
| | 2683 | CD1 | LEU | 290 | 114.357 | 40.043 | 35.951 | 1.00 | 19.53 |
| 40 | 2684 | CD2 | LEU | 290 | 116.499 | 38.741 | 35.796 | 1.00 | 18.49 |
| | 2685 | H | LEU | 290 | 117.098 | 42.681 | 33.057 | 1.00 | 25.00 |
| | 2686 | N | VAL | 291 | 116.947 | 43.857 | 36.210 | 1.00 | 27.54 |
| | 2687 | CA | VAL | 291 | 117.124 | 44.667 | 37.421 | 1.00 | 28.37 |
| | 2688 | C | VAL | 291 | 116.101 | 45.799 | 37.502 | 1.00 | 27.52 |
| 45 | 2689 | O | VAL | 291 | 115.487 | 46.023 | 38.5550 | 1.00 | 27.61 |
| | 2690 | CB | VAL | 291 | 118.544 | 45.289 | 37.507 | 1.00 | 28.94 |
| | 2691 | CG1 | VAL | 291 | 118.706 | 46.054 | 38.803 | 1.00 | 25.65 |
| | 2692 | CG2 | VAL | 291 | 119.592 | 44.214 | 37.431 | 1.00 | 36.38 |
| | 2693 | H | VAL | 291 | 117.687 | 43.782 | 35.573 | 1.00 | 25.00 |
| 50 | 2694 | N | LYS | 292 | 115.911 | 46.502 | 36.392 | 1.00 | 27.46 |
| | 2695 | CA | LYS | 292 | 114.968 | 47.611 | 36.345 | 1.00 | 28.57 |
| | 2696 | C | LYS | 292 | 113.546 | 47.158 | 36.677 | 1.00 | 30.77 |

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|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 2697 | O | LYS | 292 | 112.834 | 47.824 | 37.433 | 1.00 | 31.18 |
| | 2698 | CB | LYS | 292 | 115.029 | 48.285 | 34.976 | 1.00 | 29.35 |
| | 2699 | CG | LYS | 292 | 116.391 | 48.890 | 34.676 | 1.00 | 29.57 |
| | 2700 | CD | LYS | 292 | 116.463 | 49.431 | 33.261 | 1.00 | 34.35 |
| 5 | 2701 | CE | LYS | 292 | 117.810 | 50.079 | 32.999 | 1.00 | 37.92 |
| | 2702 | NZ | LYS | 292 | 117.909 | 50.619 | 31.619 | 1.00 | 40.64 |
| | 2703 | H | LYS | 292 | 116.413 | 46.260 | 35.581 | 1.00 | 25.00 |
| | 2704 | 1HZ | LYS | 292 | 117.780 | 49.846 | 30.936 | 1.00 | 25.00 |
| | 2705 | 2HZ | LYS | 292 | 117.169 | 51.334 | 31.476 | 1.00 | 25.00 |
| 10 | 2706 | 3HZ | LYS | 292 | 118.844 | 51.052 | 31.483 | 1.00 | 25.00 |
| | 2707 | N | THR | 293 | 113.146 | 46.010 | 36.137 | 1.00 | 34.24 |
| | 2708 | CA | THR | 293 | 111.817 | 45.463 | 36.395 | 1.00 | 27.43 |
| | 2709 | C | THR | 293 | 111.657 | 45.123 | 37.872 | 1.00 | 31.58 |
| | 2710 | O | THR | 293 | 110.655 | 45.493 | 38.491 | 1.00 | 28.71 |
| 15 | 2711 | CB | THR | 293 | 111.561 | 44.214 | 35.534 | 1.00 | 25.43 |
| | 2712 | OG1 | THR | 293 | 111.354 | 44.616 | 34.175 | 1.00 | 30.49 |
| | 2713 | CG2 | THR | 293 | 110.348 | 43.433 | 36.029 | 1.00 | 22.44 |
| | 2714 | H | THR | 293 | 113.756 | 45.525 | 35.533 | 1.00 | 25.00 |
| | 2715 | HG1 | THR | 293 | 110.577 | 45.180 | 34.129 | 1.00 | 25.00 |
| 20 | 2716 | N | ILE | 294 | 112.647 | 44.439 | 38.440 | 1.00 | 30.35 |
| | 2717 | CA | ILE | 294 | 112.596 | 44.064 | 39.853 | 1.00 | 30.45 |
| | 2718 | C | ILE | 294 | 112.481 | 45.317 | 40.725 | 1.00 | 28.69 |
| | 2719 | O | ILE | 294 | 111.709 | 45.348 | 41.685 | 1.00 | 30.57 |
| | 2720 | CB | ILE | 294 | 113.837 | 43.230 | 40.272 | 1.00 | 29.95 |
| 25 | 2721 | CG1 | ILE | 294 | 113.948 | 41.977 | 39.399 | 1.00 | 24.34 |
| | 2722 | CG2 | ILE | 294 | 113.733 | 42.818 | 41.734 | 1.00 | 18.35 |
| | 2723 | CD1 | ILE | 294 | 115.165 | 41.133 | 39.687 | 1.00 | 30.84 |
| | 2724 | H | ILE | 294 | 113.432 | 44.182 | 37.906 | 1.00 | 25.00 |
| | 2725 | N | SER | 295 | 113.219 | 46.361 | 40.359 | 1.00 | 32.61 |
| 30 | 2726 | CA | SER | 295 | 113.196 | 47.623 | 41.097 | 1.00 | 37.07 |
| | 2727 | C | SER | 295 | 111.820 | 48.276 | 41.002 | 1.00 | 35.65 |
| | 2728 | O | SER | 295 | 111.227 | 48.673 | 42.011 | 1.00 | 33.09 |
| | 2729 | CB | SER | 295 | 114.246 | 48.584 | 40.533 | 1.00 | 35.83 |
| | 2730 | OG | SER | 295 | 115.543 | 48.024 | 40.608 | 1.00 | 42.38 |
| 35 | 2731 | H | SER | 295 | 113.804 | 46.290 | 39.575 | 1.00 | 25.00 |
| | 2732 | HG | SER | 295 | 115.756 | 47.823 | 41.523 | 1.00 | 25.00 |
| | 2733 | N | MET | 296 | 111.306 | 48.342 | 39.779 | 1.00 | 34.54 |
| | 2734 | CA | MET | 296 | 110.017 | 48.951 | 39.506 | 1.00 | 35.02 |
| | 2735 | C | MET | 296 | 108.864 | 48.263 | 40.230 | 1.00 | 36.33 |
| 40 | 2736 | O | MET | 296 | 108.080 | 48.919 | 40.923 | 1.00 | 35.61 |
| | 2737 | CB | MET | 296 | 109.768 | 48.966 | 37.999 | 1.00 | 39.18 |
| | 2738 | CG | MET | 296 | 109.109 | 50.234 | 37.507 | 1.00 | 49.37 |
| | 2739 | SD | MET | 296 | 109.993 | 51.708 | 38.067 | 1.00 | 51.57 |
| | 2740 | CE | MET | 296 | 108.888 | 52.271 | 39.359 | 1.00 | 53.40 |
| 45 | 2741 | H | MET | 296 | 111.819 | 47.966 | 39.036 | 1.00 | 25.00 |
| | 2742 | N | ILE | 297 | 108.780 | 46.941 | 40.103 | 1.00 | 37.42 |
| | 2743 | CA | ILE | 297 | 107.709 | 46.185 | 40.745 | 1.00 | 34.54 |
| | 2744 | C | ILE | 297 | 107.813 | 46.267 | 42.267 | 1.00 | 36.45 |
| | 2745 | O | ILE | 297 | 106.817 | 46.101 | 42.976 | 1.00 | 35.56 |
| 50 | 2746 | CB | ILE | 297 | 107.675 | 44.709 | 40.265 | 1.00 | 36.67 |
| | 2747 | CG1 | ILE | 297 | 106.342 | 44.059 | 40.648 | 1.00 | 30.90 |
| | 2748 | CG2 | ILE | 297 | 108.858 | 43.925 | 40.821 | 1.00 | 34.15 |

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|----|-------|-----|-----|-----|----------|--------|--------|--------|-------|
| | 2749 | CD1 | ILE | 297 | 105.135 | 44.654 | 39.935 | 1.00 | 28.47 |
| | 2750 | H | ILE | 297 | 109.454 | 46.468 | 39.576 | 1.00 | 25.00 |
| | 2751 | N | SER | 298 | 109.015 | 46.559 | 42.761 | 1.00 | 37.95 |
| 5 | 2752 | CA | SER | 298 | 109.250 | 46.696 | 44.195 | 1.00 | 40.22 |
| | 2753 | C | SER | 298 | 108.531 | 47.961 | 44.673 | 1.00 | 38.96 |
| | 2754 | O | SER | 298 | 107.934 | 47.979 | 45.753 | 1.00 | 36.43 |
| | 2755 | CB | SER | 298 | 110.751 | 46.791 | 44.481 | 1.00 | 43.72 |
| | 2756 | OG | SER | 298 | 111.00 | 9 | 46.764 | 45.873 | 1.00 |
| | 62.08 | | | | | | | | |
| 10 | 2757 | H | SER | 298 | 109.775 | 46.674 | 42.153 | 1.00 | 25.00 |
| | 2758 | HG | SER | 298 | 110.573 | 47.504 | 46.304 | 1.00 | 25.00 |
| | 2759 | N | ILE | 299 | 108.582 | 49.011 | 43.857 | 1.00 | 39.57 |
| | 2760 | CA | ILE | 299 | 107.912 | 50.271 | 44.175 | 1.00 | 40.91 |
| | 2761 | C | ILE | 299 | 106.412 | 49.996 | 44.293 | 1.00 | 40.75 |
| 15 | 2762 | O | ILE | 299 | 105.771 | 50.378 | 45.276 | 1.00 | 40.26 |
| | 2763 | CB | ILE | 299 | 108.128 | 51.329 | 43.060 | 1.00 | 37.27 |
| | 2764 | CG1 | ILE | 299 | 109.614 | 51.653 | 42.908 | 1.00 | 37.90 |
| | 2765 | CG2 | ILE | 299 | 1077.345 | 52.592 | 43.370 | 1.00 | 42.54 |
| | 2766 | CD1 | ILE | 299 | 110.260 | 52.146 | 44.173 | 1.00 | 39.79 |
| 20 | 2767 | H | ILE | 299 | 109.091 | 48.942 | 43.021 | 1.00 | 25.00 |
| | 2768 | N | VAL | 300 | 105.876 | 49.290 | 43.301 | 1.00 | 34.47 |
| | 2769 | CA | VAL | 300 | 104.462 | 48.949 | 43.267 | 1.00 | 33.70 |
| | 2770 | C | VAL | 300 | 104.050 | 48.145 | 44.497 | 1.00 | 38.81 |
| | 2771 | O | VAL | 300 | 103.020 | 48.431 | 45.116 | 1.00 | 39.02 |
| 25 | 2772 | CB | VAL | 300 | 104.116 | 48.166 | 41.990 | 1.00 | 35.45 |
| | 2773 | CG1 | VAL | 300 | 102.629 | 47.848 | 41.951 | 1.00 | 37.16 |
| | 2774 | CG2 | VAL | 300 | 104.522 | 48.970 | 40.762 | 1.00 | 29.01 |
| | 2775 | H | VAL | 300 | 106.459 | 48.994 | 42.572 | 1.00 | 25.00 |
| | 2776 | N | ASP | 301 | 104.866 | 47.162 | 44.865 | 1.00 | 39.28 |
| 30 | 2777 | CA | ASP | 301 | 104.585 | 46.327 | 46.030 | 1.00 | 39.76 |
| | 2778 | C | ASP | 301 | 104.477 | 47.200 | 47.281 | 1.00 | 43.93 |
| | 2779 | O | ASP | 301 | 103.588 | 47.002 | 48.113 | 1.00 | 43.98 |
| | 2780 | CB | ASP | 301 | 105.684 | 45.270 | 46.205 | 1.00 | 41.93 |
| | 2781 | CG | ASP | 301 | 105.401 | 44.299 | 47.348 | 1.00 | 47.18 |
| 35 | 2782 | OD1 | ASP | 301 | 104.219 | 44.006 | 47.633 | 1.00 | 52.50 |
| | 2783 | OD2 | ASP | 301 | 106.375 | 43.817 | 47.959 | 1.00 | 53.58 |
| | 2784 | H | ASP | 301 | 105.672 | 46.984 | 44.338 | 1.00 | 25.00 |
| | 2785 | N | ASP | 302 | 105.373 | 48.175 | 47.401 | 1.00 | 48.10 |
| | 2786 | CA | ASP | 302 | 105.371 | 49.088 | 48.541 | 1.00 | 51.62 |
| 40 | 2787 | C | ASP | 302 | 104.090 | 49.918 | 48.560 | 1.00 | 50.46 |
| | 2788 | O | ASP | 302 | 103.480 | 50.114 | 49.615 | 1.00 | 51.17 |
| | 2789 | CB | ASP | 302 | 106.587 | 50.017 | 48.487 | 1.00 | 55.75 |
| | 2790 | CG | ASP | 302 | 107.904 | 49.271 | 48.619 | 1.00 | 62.15 |
| | 2791 | OD1 | ASP | 302 | 107.922 | 48.165 | 49.207 | 1.00 | 63.08 |
| 45 | 2792 | OD2 | ASP | 302 | 108.928 | 49.798 | 48.133 | 1.00 | 68.25 |
| | 2793 | H | ASP | 302 | 106.056 | 48.281 | 46.704 | 1.00 | 25.00 |
| | 2794 | N | THR | 303 | 103.684 | 50.388 | 47.383 | 1.00 | 50.52 |
| | 2795 | CA | THR | 303 | 102.479 | 51.192 | 47.230 | 1.00 | 50.05 |
| | 2796 | C | THR | 303 | 101.260 | 50.472 | 47.808 | 1.00 | 51.84 |
| 50 | 2797 | O | THR | 303 | 100.563 | 51.013 | 48.668 | 1.00 | 56.07 |
| | 2798 | CB | THR | 303 | 102.222 | 51.512 | 45.745 | 1.00 | 50.09 |
| | 2799 | OG1 | THR | 303 | 103.377 | 52.153 | 45.190 | 1.00 | 45.79 |

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|----|------|-----|-----|-----|---------|--------|--------|------|--------|
| | 2800 | CG2 | THR | 303 | 101.015 | 52.425 | 45.593 | 1.00 | 50.31 |
| | 2801 | H | THR | 303 | 104.219 | 50.190 | 46.581 | 1.00 | 25.00 |
| | 2802 | HG1 | THR | 303 | 103.480 | 52.938 | 45.719 | 1.00 | 25.00 |
| | 2803 | N | PHE | 304 | 101.025 | 49.246 | 47.352 | 1.00 | 50.29 |
| 5 | 2804 | CA | PHE | 304 | 99.893 | 48.450 | 47.817 | 1.00 | 53.29 |
| | 2805 | C | PHE | 304 | 99.997 | 48.024 | 49.275 | 1.00 | 59.68 |
| | 2806 | O | PHE | 304 | 98.981 | 47.832 | 49.940 | 1.00 | 62.17 |
| | 2807 | CB | PHE | 304 | 99.744 | 47.182 | 46.971 | 1.00 | 43.62 |
| | 2808 | CG | PHE | 304 | 99.065 | 47.398 | 45.654 | 1.00 | 37.53 |
| 10 | 2809 | CD1 | PHE | 304 | 99.780 | 47.857 | 44.555 | 1.00 | 32.17 |
| | 2810 | CD2 | PHE | 304 | 97.711 | 47.113 | 45.506 | 1.00 | 35.92 |
| | 2811 | CE1 | PHE | 304 | 99.156 | 48.029 | 43.326 | 1.00 | 36.26 |
| | 2812 | CE2 | PHE | 304 | 97.079 | 47.280 | 44.283 | 1.00 | 29.26 |
| | 2813 | CZ | PHE | 304 | 97.802 | 47.739 | 43.189 | 1.00 | 34.73 |
| 15 | 2814 | H | PHE | 304 | 101.636 | 48.860 | 46.683 | 1.00 | 25.00 |
| | 2815 | N | ASP | 305 | 101.223 | 47.873 | 49.765 | 1.00 | 69.36 |
| | 2816 | CA | ASP | 305 | 101.450 | 47.405 | 51.129 | 1.00 | 78.46 |
| | 2817 | C | ASP | 305 | 101.326 | 48.406 | 52.279 | 1.00 | 80.92 |
| | 2818 | O | ASP | 305 | 100.774 | 48.064 | 53.329 | 1.00 | 79.13 |
| 20 | 2819 | CB | ASP | 305 | 102.798 | 46.675 | 51.210 | 1.00 | 84.84 |
| | 2820 | CG | ASP | 305 | 102.851 | 45.663 | 52.345 | 1.00 | 90.63 |
| | 2821 | OD1 | ASP | 305 | 102.142 | 44.635 | 52.265 | 1.00 | 90.70 |
| | 2822 | OD2 | ASP | 305 | 103.610 | 45.891 | 53.312 | 1.00 | 92.23 |
| | 2823 | H | ASP | 305 | 101.996 | 48.072 | 49.197 | 1.00 | 25.00 |
| 25 | 2824 | N | ALA | 306 | 101.818 | 49.631 | 52.104 | 1.00 | 84.70 |
| | 2825 | CA | ALA | 306 | 101.752 | 50.595 | 53.201 | 1.00 | 89.65 |
| | 2826 | C | ALA | 306 | 101.457 | 52.057 | 52.874 | 1.00 | 91.11 |
| | 2827 | O | ALA | 306 | 101.606 | 52.916 | 53.745 | 1.00 | 93.41 |
| | 2828 | CB | ALA | 306 | 103.027 | 50.500 | 54.040 | 1.00 | 89.50 |
| 30 | 2829 | H | ALA | 306 | 102.229 | 49.879 | 51.249 | 1.00 | 25.00 |
| | 2830 | N | TYR | 307 | 101.022 | 52.359 | 51.655 | 1.00 | 90.94 |
| | 2831 | CA | TYR | 307 | 100.743 | 53.752 | 51.329 | 1.00 | 92.48 |
| | 2832 | C | TYR | 307 | 99.374 | 54.011 | 50.701 | 1.00 | 90.37 |
| | 2833 | O | TYR | 307 | 98.599 | 54.824 | 51.207 | 1.00 | 91.55 |
| 35 | 2834 | CB | TYR | 307 | 101.858 | 54.336 | 50.453 | 1.00 | 98.27 |
| | 2835 | CG | TYR | 307 | 102.031 | 55.837 | 50.609 | 1.00 | 106.75 |
| | 2836 | CD1 | TYR | 307 | 101.301 | 56.732 | 49.825 | 1.00 | 109.71 |
| | 2837 | CD2 | TYR | 307 | 102.918 | 56.364 | 51.552 | 1.00 | 107.24 |
| | 2838 | CE1 | TYR | 307 | 101.447 | 58.113 | 49.973 | 1.00 | 107.24 |
| 40 | 2839 | CE2 | TYR | 307 | 103.072 | 57.744 | 51.708 | 1.00 | 106.57 |
| | 2840 | CZ | TYR | 307 | 102.332 | 58.611 | 50.915 | 1.00 | 106.75 |
| | 2841 | OH | TYR | 307 | 102.477 | 59.971 | 51.060 | 1.00 | 103.97 |
| | 2842 | H | TYR | 307 | 100.876 | 51.657 | 50.988 | 1.00 | 25.00 |
| | 2843 | HH | TYR | 307 | 101.900 | 60.427 | 50.443 | 1.00 | 25.00 |
| 45 | 2844 | N | GLY | 308 | 99.079 | 53.325 | 49.603 | 1.00 | 85.79 |
| | 2845 | CA | GLY | 308 | 97.808 | 53.522 | 48.930 | 1.00 | 82.54 |
| | 2846 | C | GLY | 308 | 96.583 | 53.120 | 49.730 | 1.00 | 81.67 |
| | 2847 | O | GLY | 308 | 96.589 | 52.105 | 50.428 | 1.00 | 80.43 |
| | 2848 | H | GLY | 308 | 99.710 | 52.666 | 49.258 | 1.00 | 25.00 |
| 50 | 2849 | N | THR | 309 | 95.531 | 53.928 | 49.637 | 1.00 | 82.42 |
| | 2850 | CA | THR | 309 | 94.282 | 53.649 | 50.338 | 1.00 | 82.64 |
| | 2851 | C | THR | 309 | 93.397 | 52.796 | 49.433 | 1.00 | 83.27 |

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|----|------|-----|-----|-----|--------|--------|--------|------|--------|
| | 2852 | O | THR | 309 | 93.592 | 52.771 | 48.215 | 1.00 | 87.28 |
| | 2853 | CB | THR | 309 | 93.519 | 54.946 | 50.696 | 1.00 | 80.48 |
| | 2854 | OG1 | THR | 309 | 93.166 | 55.648 | 49.495 | 1.00 | 74.90 |
| | 2855 | CG2 | THR | 309 | 94.371 | 55.844 | 51.583 | 1.00 | 75.37 |
| 5 | 2856 | H | THR | 309 | 95.600 | 54.729 | 49.085 | 1.00 | 25.00 |
| | 2857 | HG1 | THR | 309 | 92.598 | 55.106 | 48.954 | 1.00 | 25.00 |
| | 2858 | N | VAL | 310 | 92.383 | 52.172 | 50.025 | 1.00 | 80.18 |
| | 2859 | CA | VAL | 310 | 91.447 | 51.304 | 49.309 | 1.00 | 75.06 |
| | 2860 | C | VAL | 310 | 91.067 | 51.822 | 47.919 | 1.00 | 74.05 |
| 10 | 2861 | O | VAL | 310 | 91.209 | 51.115 | 46.921 | 1.00 | 73.13 |
| | 2862 | CB | VAL | 310 | 90.149 | 51.103 | 50.127 | 1.00 | 79.21 |
| | 2863 | CG1 | VAL | 310 | 89.284 | 50.020 | 49.494 | 1.00 | 80.28 |
| | 2864 | CG2 | VAL | 310 | 90.478 | 50.760 | 51.575 | 1.00 | 78.07 |
| | 2865 | H | VAL | 310 | 92.275 | 52.293 | 50.987 | 1.00 | 25.00 |
| 15 | 2866 | N | LYS | 311 | 90.622 | 53.072 | 47.859 | 1.00 | 73.34 |
| | 2867 | CA | LYS | 311 | 90.210 | 53.682 | 46.600 | 1.00 | 71.58 |
| | 2868 | C | LYS | 311 | 91.366 | 53.946 | 45.639 | 1.00 | 67.72 |
| | 2869 | O | LYS | 311 | 91.269 | 53.642 | 44.448 | 1.00 | 65.13 |
| | 2870 | CB | LYS | 311 | 89.433 | 54.977 | 46.866 | 1.00 | 79.85 |
| 20 | 2871 | CG | LYS | 311 | 87.977 | 54.774 | 47.306 | 1.00 | 89.57 |
| | 2872 | CD | LYS | 311 | 87.842 | 53.976 | 48.607 | 1.00 | 98.38 |
| | 2873 | CE | LYS | 311 | 88.473 | 54.694 | 49.795 | 1.00 | 102.39 |
| | 2874 | NZ | LYS | 311 | 87.808 | 55.997 | 50.082 | 1.00 | 107.12 |
| | 2875 | H | LYS | 311 | 90.572 | 53.594 | 48.679 | 1.00 | 25.00 |
| 25 | 2876 | 1HZ | LYS | 311 | 87.884 | 56.617 | 49.250 | 1.00 | 25.00 |
| | 2877 | 2HZ | LYS | 311 | 86.804 | 55.833 | 50.299 | 1.00 | 25.00 |
| | 2878 | 3HZ | LYS | 311 | 88.268 | 56.452 | 50.896 | 1.00 | 25.00 |
| | 2879 | N | GLU | 312 | 92.461 | 54.495 | 46.162 | 1.00 | 64.41 |
| | 2880 | CA | GLU | 312 | 93.634 | 54.805 | 45.346 | 1.00 | 61.39 |
| 30 | 2881 | C | GLU | 312 | 94.189 | 53.556 | 44.667 | 1.00 | 61.26 |
| | 2882 | O | GLU | 312 | 94.533 | 53.585 | 43.483 | 1.00 | 59.48 |
| | 2883 | CB | GLU | 312 | 94.724 | 55.465 | 46.194 | 1.00 | 63.39 |
| | 2884 | CG | GLU | 312 | 94.348 | 56.830 | 46.748 | 1.00 | 70.79 |
| | 2885 | CD | GLU | 312 | 95.456 | 57.456 | 47.578 | 1.00 | 75.21 |
| 35 | 2886 | OE1 | GLU | 312 | 95.879 | 56.840 | 48.579 | 1.00 | 77.19 |
| | 2887 | OE2 | GLU | 312 | 95.903 | 58.570 | 47.233 | 1.00 | 79.86 |
| | 2888 | H | GLU | 312 | 92.482 | 54.687 | 47.112 | 1.00 | 25.00 |
| | 2889 | N | LEU | 313 | 94.257 | 52.459 | 45.418 | 1.00 | 57.55 |
| | 2890 | CA | LEU | 313 | 94.765 | 51.198 | 44.891 | 1.00 | 52.69 |
| 40 | 2891 | C | LEU | 313 | 93.885 | 50.678 | 43.762 | 1.00 | 52.82 |
| | 2892 | O | LEU | 313 | 94.391 | 50.281 | 42.713 | 1.00 | 51.15 |
| | 2893 | CB | LEU | 313 | 94.883 | 50.158 | 46.005 | 1.00 | 48.63 |
| | 2894 | CG | LEU | 313 | 95.886 | 50.519 | 47.102 | 1.00 | 46.47 |
| | 2895 | CD1 | LEU | 313 | 95.941 | 49.416 | 48.140 | 1.00 | 48.38 |
| 45 | 2896 | CD2 | LEU | 313 | 97.259 | 50.748 | 46.495 | 1.00 | 48.00 |
| | 2897 | H | LEU | 313 | 93.952 | 52.495 | 46.346 | 1.00 | 25.00 |
| | 2898 | N | GLU | 314 | 92.569 | 50.724 | 43.957 | 1.00 | 52.92 |
| | 2899 | CA | GLU | 314 | 91.634 | 50.269 | 42.933 | 1.00 | 54.92 |
| | 2900 | C | GLU | 314 | 91.840 | 51.087 | 41.651 | 1.00 | 52.05 |
| 50 | 2901 | O | GLU | 314 | 91.801 | 50.548 | 40.541 | 1.00 | 49.73 |
| | 2902 | CB | GLU | 314 | 90.189 | 50.400 | 43.431 | 1.00 | 58.82 |
| | 2903 | CG | GLU | 314 | 89.137 | 49.809 | 42.488 | 1.00 | 68.28 |

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|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 2904 | CD | GLU | 314 | 89.281 | 48.303 | 42.292 | 1.00 | 74.40 |
| | 2905 | OE1 | GLU | 314 | 89.097 | 47.550 | 43.275 | 1.00 | 76.74 |
| | 2906 | OE2 | GLU | 314 | 89.568 | 47.871 | 41.152 | 1.00 | 74.09 |
| | 2907 | H | GLU | 314 | 92.221 | 51.057 | 44.810 | 1.00 | 25.00 |
| 5 | 2908 | N | ALA | 315 | 92.088 | 52.383 | 41.813 | 1.00 | 51.92 |
| | 2909 | CA | ALA | 315 | 92.323 | 53.270 | 40.678 | 1.00 | 54.57 |
| | 2910 | C | ALA | 315 | 93.649 | 52.920 | 39.993 | 1.00 | 51.51 |
| | 2911 | O | ALA | 315 | 93.762 | 52.977 | 38.763 | 1.00 | 49.98 |
| | 2912 | CB | ALA | 315 | 92.335 | 54.722 | 41.142 | 1.00 | 52.19 |
| 10 | 2913 | H | ALA | 315 | 92.103 | 52.753 | 42.723 | 1.00 | 25.00 |
| | 2914 | N | TYR | 316 | 94.640 | 52.542 | 40.796 | 1.00 | 49.90 |
| | 2915 | CA | TYR | 316 | 95.960 | 52.177 | 40.289 | 1.00 | 46.00 |
| | 2916 | C | TYR | 316 | 95.911 | 50.864 | 39.506 | 1.00 | 42.05 |
| | 2917 | O | TYR | 316 | 96.503 | 50.756 | 38.424 | 1.00 | 36.96 |
| 15 | 2918 | CB | TYR | 316 | 96.954 | 52.070 | 41.445 | 1.00 | 48.32 |
| | 2919 | CG | TYR | 316 | 98.405 | 52.154 | 41.029 | 1.00 | 52.17 |
| | 2920 | CD1 | TYR | 316 | 98.975 | 53.371 | 40.657 | 1.00 | 53.66 |
| | 2921 | CD2 | TYR | 316 | 99.218 | 51.023 | 41.033 | 1.00 | 58.41 |
| | 2922 | CE1 | TYR | 316 | 100.320 | 53.461 | 40.303 | 1.00 | 56.28 |
| 20 | 2923 | CE2 | TYR | 316 | 100.566 | 51.101 | 40.681 | 1.00 | 63.22 |
| | 2924 | CZ | TYR | 316 | 101.110 | 52.323 | 40.319 | 1.00 | 58.59 |
| | 2925 | OH | TYR | 316 | 102.442 | 52.405 | 39.986 | 1.00 | 51.77 |
| | 2926 | H | TYR | 316 | 94.483 | 52.514 | 41.763 | 1.00 | 25.00 |
| | 2927 | HH | TYR | 316 | 102.631 | 53.311 | 39.758 | 1.00 | 25.00 |
| 25 | 2928 | N | THR | 317 | 95.186 | 49.881 | 40.040 | 1.00 | 38.98 |
| | 2929 | CA | THR | 317 | 95.044 | 48.574 | 39.396 | 1.00 | 40.08 |
| | 2930 | C | THR | 317 | 94.391 | 48.732 | 38.025 | 1.00 | 41.19 |
| | 2931 | O | THR | 317 | 94.755 | 48.046 | 37.065 | 1.00 | 40.64 |
| | 2932 | CB | THR | 317 | 94.189 | 47.619 | 40.245 | 1.00 | 39.21 |
| 30 | 2933 | OG1 | THR | 317 | 94.658 | 47.632 | 41.598 | 1.00 | 40.99 |
| | 2934 | CG2 | THR | 317 | 94.277 | 46.198 | 39.698 | 1.00 | 41.75 |
| | 2935 | H | THR | 317 | 94.740 | 50.022 | 40.900 | 1.00 | 25.00 |
| | 2936 | HG1 | THR | 317 | 94.120 | 47.056 | 42.134 | 1.00 | 25.00 |
| | 2937 | N | ASP | 318 | 93.423 | 49.641 | 37.945 | 1.00 | 46.22 |
| 35 | 2938 | CA | ASP | 318 | 92.719 | 49.920 | 36.700 | 1.00 | 44.99 |
| | 2939 | C | ASP | 318 | 93.631 | 50.595 | 35.693 | 1.00 | 38.74 |
| | 2940 | O | ASP | 318 | 93.695 | 50.183 | 34.536 | 1.00 | 39.12 |
| | 2941 | CB | ASP | 318 | 91.497 | 50.799 | 36.959 | 1.00 | 55.80 |
| | 2942 | CG | ASP | 318 | 90.215 | 50.006 | 36.977 | 1.00 | 64.67 |
| 40 | 2943 | OD1 | ASP | 318 | 89.924 | 49.364 | 38.010 | 1.00 | 73.33 |
| | 2944 | OD2 | ASP | 318 | 89.507 | 50.014 | 35.948 | 1.00 | 72.06 |
| | 2945 | H | ASP | 318 | 93.171 | 50.138 | 38.755 | 1.00 | 25.00 |
| | 2946 | N | ALA | 319 | 94.340 | 51.628 | 36.135 | 1.00 | 37.74 |
| | 2947 | CA | ALA | 319 | 95.258 | 52.347 | 35.260 | 1.00 | 40.21 |
| 45 | 2948 | C | ALA | 319 | 96.245 | 51.360 | 34.644 | 1.00 | 42.98 |
| | 2949 | O | ALA | 319 | 96.528 | 51.422 | 33.446 | 1.00 | 41.24 |
| | 2950 | CB | ALA | 319 | 95.995 | 53.426 | 36.039 | 1.00 | 42.19 |
| | 2951 | H | ALA | 319 | 94.240 | 51.923 | 37.067 | 1.00 | 25.00 |
| | 2952 | N | ILE | 320 | 96.727 | 50.423 | 35.462 | 1.00 | 41.94 |
| 50 | 2953 | CA | ILE | 320 | 97.670 | 49.403 | 35.005 | 1.00 | 40.80 |
| | 2954 | C | ILE | 320 | 97.064 | 48.488 | 33.934 | 1.00 | 37.20 |
| | 2955 | O | ILE | 320 | 97.711 | 48.200 | 32.923 | 1.00 | 31.26 |

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|----|-------|------|-----|-----|---------|--------|--------|------|-------|
| | 2956 | CB | ILE | 320 | 98.198 | 48.549 | 36.191 | 1.00 | 40.22 |
| | 2957 | CG1 | ILE | 320 | 99.093 | 49.404 | 37.091 | 1.00 | 38.13 |
| | 2958 | CG2 | ILE | 320 | 98.973 | 47.332 | 35.680 | 1.00 | 36.19 |
| | 2959 | CD1 | ILE | 320 | 100.340 | 49.924 | 36.392 | 1.00 | 35.64 |
| 5 | 2960 | H | ILE | 320 | 96.447 | 50.429 | 36.402 | 1.00 | 25.00 |
| | 2961 | N | GLN | 321 | 95.830 | 48.037 | 34.149 | 1.00 | 37.70 |
| | 2962 | CA | GLN | 321 | 95.167 | 47.161 | 33.180 | 1.00 | 43.79 |
| | 2963 | C | GLN | 321 | 94.959 | 47.867 | 31.839 | 1.00 | 44.60 |
| | 2964 | O | GLN | 321 | 95.104 | 47.254 | 30.777 | 1.00 | 43.29 |
| 10 | 2965 | CB | GLN | 321 | 93.818 | 46.662 | 33.713 | 1.00 | 45.39 |
| | 2966 | CG | GLN | 321 | 93.879 | 45.997 | 35.079 | 1.00 | 50.49 |
| | 2967 | CD | GLN | 321 | 94.981 | 44.963 | 35.182 | 1.00 | 52.12 |
| | 2968 | OE1 | GLN | 321 | 95.097 | 44.073 | 34.341 | 1.00 | 53.96 |
| | 2969 | NE2 | GLN | 321 | 95.801 | 45.078 | 36.220 | 1.00 | 49.92 |
| 15 | 2970 | H | GLN | 321 | 95.360 | 48.301 | 34.967 | 1.00 | 25.00 |
| | 2971 | 1HE2 | GLN | 321 | 96.511 | 44.405 | 36.295 | 1.00 | 25.00 |
| | 2972 | 2HE2 | GLN | 321 | 95.664 | 45.810 | 36.855 | 1.00 | 25.00 |
| | 2973 | N | ARG | 322 | 94.595 | 49.148 | 31.894 | 1.00 | 48.28 |
| | 2974 | CA | ARG | 322 | 94.376 | 49.935 | 30.683 | 1.00 | 48.66 |
| 20 | 2975 | C | ARG | 322 | 95.697 | 50.181 | 29.976 | 1.00 | 48.74 |
| | 2976 | O | ARG | 322 | 95.756 | 50.167 | 28.745 | 1.00 | 52.54 |
| | 2977 | CB | ARG | 322 | 93.701 | 51.272 | 31.003 | 1.00 | 53.96 |
| | 2978 | CG | ARG | 322 | 92.175 | 51.230 | 31.029 | 1.00 | 62.97 |
| | 2979 | CD | ARG | 322 | 91.642 | 50.367 | 32.164 | 1.00 | 68.65 |
| 25 | 29880 | NE | ARG | 322 | 90.183 | 50.288 | 32.167 | 1.00 | 71.23 |
| | 2981 | CZ | ARG | 322 | 89.377 | 51.274 | 32.546 | 1.00 | 73.12 |
| | 2982 | NH1 | ARG | 322 | 89.878 | 52.432 | 32.959 | 1.00 | 75.57 |
| | 2983 | NH2 | ARG | 322 | 88.064 | 51.101 | 32.512 | 1.00 | 75.20 |
| | 2984 | H | ARG | 322 | 94.477 | 49.570 | 32.771 | 1.00 | 25.00 |
| 30 | 2985 | HE | ARG | 322 | 83.771 | 49.449 | 31.873 | 1.00 | 25.00 |
| | 2986 | 1HH1 | ARG | 322 | 90.868 | 52.574 | 32.983 | 1.00 | 25.00 |
| | 2987 | 2HH1 | ARG | 322 | 89.263 | 53.172 | 33.235 | 1.00 | 25.00 |
| | 2988 | 1HH2 | ARG | 322 | 87.684 | 50.229 | 32.203 | 1.00 | 25.00 |
| | 2989 | 2HH2 | ARG | 322 | 87.455 | 51.842 | 32.793 | 1.00 | 25.00 |
| 35 | 2990 | N | TRP | 323 | 96.740 | 50.434 | 30.765 | 1.00 | 48.78 |
| | 2991 | CA | TRP | 323 | 98.086 | 50.674 | 30.248 | 1.00 | 50.53 |
| | 2992 | C | TRP | 323 | 98.036 | 51.721 | 29.139 | 1.00 | 51.62 |
| | 2993 | O | TRP | 323 | 98.368 | 51.442 | 27.984 | 1.00 | 46.60 |
| | 2994 | CB | TRP | 323 | 98.676 | 49.361 | 29.719 | 1.00 | 45.66 |
| 40 | 2995 | CG | TRP | 323 | 100.171 | 49.334 | 29.673 | 1.00 | 43.84 |
| | 2996 | CD1 | TRP | 323 | 100.972 | 49.778 | 28.660 | 1.00 | 41.07 |
| | 2997 | CD2 | TRP | 323 | 101.045 | 48.811 | 30.677 | 1.00 | 42.00 |
| | 2998 | NE1 | TRP | 323 | 102.292 | 49.559 | 28.969 | 1.00 | 41.37 |
| | 2999 | CE2 | TRP | 323 | 102.367 | 48.967 | 30.202 | 1.00 | 42.95 |
| 45 | 3000 | CE3 | TRP | 323 | 100.841 | 48.222 | 31.932 | 1.00 | 43.56 |
| | 3001 | CZ2 | TRP | 323 | 103.483 | 48.555 | 30.939 | 1.00 | 41.64 |
| | 3002 | CZ3 | TRP | 323 | 101.952 | 47.812 | 32.666 | 1.00 | 46.00 |
| | 3003 | CH2 | TRP | 323 | 103.256 | 47.982 | 32.164 | 1.00 | 42.99 |
| | 3004 | H | TRP | 323 | 96.604 | 50.455 | 31.735 | 1.00 | 25.00 |
| 50 | 3005 | HE1 | TRP | 323 | 103.052 | 49.790 | 28.396 | 1.00 | 25.00 |
| | 3006 | N | ASP | 324 | 97.624 | 52.931 | 29.503 | 1.00 | 59.55 |
| | 3007 | CA | ASP | 324 | 97.500 | 54.015 | 28.539 | 1.00 | 65.59 |

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|----|------|------|-----|-----|---------|--------|--------|------|-------|
| | 3008 | C | ASP | 324 | 98.480 | 55.143 | 28.844 | 1.00 | 64.51 |
| | 3009 | O | ASP | 324 | 99.591 | 55.176 | 28.316 | 1.00 | 68.35 |
| | 3010 | CB | ASP | 324 | 96.056 | 54.541 | 28.552 | 1.00 | 70.35 |
| | 3011 | CG | ASP | 324 | 95.713 | 55.365 | 27.320 | 1.00 | 74.75 |
| 5 | 3012 | OD1 | ASP | 324 | 96.439 | 56.333 | 27.008 | 1.00 | 77.92 |
| | 3013 | OD2 | ASP | 324 | 94.698 | 55.043 | 26.668 | 1.00 | 77.68 |
| | 3014 | H | ASP | 324 | 97.422 | 53.067 | 30.447 | 1.00 | 25.00 |
| | 3015 | N | ILE | 325 | 98.025 | 56.067 | 29.685 | 1.00 | 59.63 |
| | 3016 | CA | ILE | 325 | 98.765 | 57.248 | 30.131 | 1.00 | 62.22 |
| 10 | 3017 | C | ILE | 325 | 97.699 | 58.281 | 30.472 | 1.00 | 62.36 |
| | 3018 | O | ILE | 325 | 97.807 | 58.988 | 31.467 | 1.00 | 57.92 |
| | 3019 | CB | ILE | 325 | 99.752 | 57.824 | 29.066 | 1.00 | 58.28 |
| | 3020 | CG1 | ILE | 325 | 100.656 | 58.874 | 29.713 | 1.00 | 56.91 |
| | 3021 | CG2 | ILE | 325 | 99.004 | 58.424 | 27.882 | 1.00 | 53.60 |
| 15 | 3022 | CD1 | ILE | 325 | 101.760 | 59.364 | 28.812 | 1.00 | 65.51 |
| | 3023 | H | ILE | 325 | 97.138 | 55.950 | 30.059 | 1.00 | 25.00 |
| | 3024 | N | ASN | 326 | 96.622 | 58.287 | 29.687 | 1.00 | 64.69 |
| | 3025 | CA | ASN | 326 | 95.504 | 59.203 | 29.902 | 1.00 | 68.20 |
| | 3026 | C | ASN | 326 | 94.857 | 58.860 | 31.238 | 1.00 | 71.30 |
| 20 | 3027 | O | ASN | 326 | 94.171 | 59.684 | 31.846 | 1.00 | 76.27 |
| | 3028 | CB | ASN | 326 | 94.462 | 59.058 | 28.787 | 1.00 | 67.58 |
| | 3029 | CG | ASN | 326 | 95.041 | 59.297 | 27.406 | 1.00 | 69.04 |
| | 3030 | OD1 | ASN | 326 | 96.055 | 59.975 | 27.225 | 1.00 | 68.18 |
| | 3031 | ND2 | ASN | 326 | 94.410 | 58.716 | 26.395 | 1.00 | 67.11 |
| 25 | 3032 | H | ASN | 326 | 96.599 | 57.685 | 28.918 | 1.00 | 25.00 |
| | 3033 | 1HD2 | ASN | 326 | 94.783 | 58.869 | 25.501 | 1.00 | 25.00 |
| | 3034 | 2HD2 | ASN | 326 | 93.618 | 58.173 | 26.568 | 1.00 | 25.00 |
| | 3035 | N | GLU | 327 | 95.095 | 57.631 | 31.691 | 1.00 | 70.98 |
| | 3036 | CA | GLU | 327 | 94.553 | 57.144 | 32.952 | 1.00 | 69.92 |
| 30 | 3037 | C | GLU | 327 | 95.259 | 57.798 | 34.138 | 1.00 | 67.58 |
| | 3038 | O | GLU | 327 | 94.751 | 57.777 | 35.260 | 1.00 | 68.23 |
| | 3039 | CB | GLU | 327 | 94.709 | 55.622 | 33.034 | 1.00 | 69.72 |
| | 3040 | CG | GLU | 327 | 94.147 | 54.858 | 31.838 | 1.00 | 66.84 |
| | 3041 | CD | GLU | 327 | 92.650 | 55.040 | 31.659 | 1.00 | 69.61 |
| 35 | 3042 | OE1 | GLU | 327 | 91.899 | 54.845 | 32.639 | 1.00 | 69.86 |
| | 3043 | OE2 | GLU | 327 | 92.225 | 55.369 | 30.530 | 1.00 | 66.87 |
| | 3044 | H | GLU | 327 | 95.646 | 57.037 | 31.159 | 1.00 | 25.00 |
| | 3045 | N | ILE | 328 | 96.411 | 58.407 | 33.872 | 1.00 | 64.07 |
| | 3046 | CA | ILE | 328 | 97.212 | 59.065 | 34.901 | 1.00 | 63.90 |
| 40 | 3047 | C | ILE | 328 | 96.425 | 60.142 | 35.657 | 1.00 | 70.44 |
| | 3048 | O | ILE | 328 | 96.624 | 60.338 | 36.857 | 1.00 | 69.65 |
| | 3049 | CB | ILE | 328 | 98.508 | 59.669 | 34.286 | 1.00 | 56.23 |
| | 3050 | CG1 | ILE | 328 | 99.578 | 59.844 | 35.359 | 1.00 | 56.00 |
| | 3051 | CG2 | ILE | 328 | 98.223 | 61.007 | 33.618 | 1.00 | 53.09 |
| 45 | 3052 | CD1 | ILE | 328 | 100.948 | 60.162 | 34.799 | 1.00 | 58.67 |
| | 3053 | H | ILE | 328 | 96.744 | 58.430 | 32.958 | 1.00 | 25.00 |
| | 3054 | N | ASP | 329 | 95.487 | 60.780 | 34.961 | 1.00 | 75.68 |
| | 3055 | CA | ASP | 329 | 94.659 | 61.844 | 35.531 | 1.00 | 79.88 |
| | 3056 | C | ASP | 329 | 93.764 | 61.377 | 36.677 | 1.00 | 79.44 |
| 50 | 3057 | O | ASP | 329 | 93.303 | 62.188 | 37.483 | 1.00 | 79.71 |
| | 3058 | CB | ASP | 329 | 93.796 | 62.476 | 34.435 | 1.00 | 85.36 |
| | 3059 | CG | ASP | 329 | 94.608 | 62.912 | 33.226 | 1.00 | 90.96 |

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|----|------|------|-----|-----|---------|--------|--------|------|-------|
| | 3060 | OD1 | ASP | 329 | 95.719 | 63.461 | 33.409 | 1.00 | 93.02 |
| | 3061 | OD2 | ASP | 329 | 94.133 | 62.699 | 32.090 | 1.00 | 93.14 |
| | 3062 | H | ASP | 329 | 95.344 | 60.527 | 34.026 | 1.00 | 25.00 |
| | 3063 | N | ARG | 330 | 93.501 | 60.074 | 36.730 | 1.00 | 76.85 |
| 5 | 3064 | CA | ARG | 330 | 92.658 | 59.501 | 37.775 | 1.00 | 75.38 |
| | 3065 | C | ARG | 330 | 93.488 | 59.059 | 38.981 | 1.00 | 71.57 |
| | 3066 | O | ARG | 330 | 92.935 | 58.631 | 39.998 | 1.00 | 69.70 |
| | 3067 | CB | ARG | 330 | 91.881 | 58.300 | 37.227 | 1.00 | 75.33 |
| | 3068 | CG | ARG | 330 | 91.177 | 58.562 | 35.905 | 1.00 | 78.99 |
| 10 | 3069 | CD | ARG | 330 | 90.383 | 57.350 | 35.454 | 1.00 | 80.32 |
| | 3070 | NE | ARG | 330 | 89.861 | 57.517 | 34.100 | 1.00 | 86.31 |
| | 3071 | CZ | ARG | 330 | 88.851 | 56.816 | 33.592 | 1.00 | 88.51 |
| | 3072 | NH1 | ARG | 330 | 88.239 | 55.894 | 34.325 | 1.00 | 91.01 |
| | 3073 | NH2 | ARG | 330 | 88.458 | 57.030 | 32.344 | 1.00 | 89.50 |
| 15 | 3074 | H | ARG | 330 | 93.891 | 59.477 | 36.060 | 1.00 | 25.00 |
| | 3075 | HE | ARG | 330 | 90.281 | 58.188 | 33.523 | 1.00 | 25.00 |
| | 3076 | 1HH1 | ARG | 330 | 88.533 | 55.723 | 35.265 | 1.00 | 25.00 |
| | 3077 | 2HH1 | ARG | 330 | 87.475 | 55.375 | 33.942 | 1.00 | 25.00 |
| | 3078 | 1HH2 | ARG | 330 | 88.917 | 57.720 | 31.786 | 1.00 | 25.00 |
| 20 | 3079 | 2HH2 | ARG | 330 | 87.692 | 56.508 | 31.966 | 1.00 | 25.00 |
| | 3080 | N | LEU | 331 | 94.809 | 59.174 | 38.867 | 1.00 | 67.63 |
| | 3081 | CA | LEU | 331 | 95.723 | 58.761 | 39.930 | 1.00 | 62.95 |
| | 3082 | C | LEU | 331 | 96.290 | 59.919 | 40.735 | 1.00 | 60.42 |
| | 3083 | O | LEU | 331 | 96.590 | 60.974 | 40.186 | 1.00 | 58.28 |
| 25 | 3084 | CB | LEU | 331 | 96.906 | 57.985 | 39.338 | 1.00 | 58.68 |
| | 3085 | CG | LEU | 331 | 96.664 | 56.739 | 38.486 | 1.00 | 54.70 |
| | 3086 | CD1 | LEU | 331 | 97.992 | 56.255 | 37.941 | 1.00 | 46.64 |
| | 3087 | CD2 | LEU | 331 | 95.988 | 55.654 | 39.304 | 1.00 | 48.82 |
| | 3088 | H | LEU | 331 | 95.195 | 59.574 | 38.061 | 1.00 | 25.00 |
| 30 | 3089 | N | PRO | 332 | 96.426 | 59.743 | 42.058 | 1.00 | 57.70 |
| | 3090 | CA | PRO | 332 | 96.981 | 60.814 | 42.886 | 1.00 | 58.87 |
| | 3091 | C | PRO | 332 | 98.455 | 60.977 | 42.521 | 1.00 | 61.32 |
| | 3092 | O | PRO | 332 | 99.132 | 59.997 | 42.207 | 1.00 | 63.75 |
| | 3093 | CB | PRO | 332 | 96.800 | 60.278 | 44.307 | 1.00 | 58.32 |
| 35 | 3094 | CG | PRO | 332 | 96.819 | 58.793 | 44.122 | 1.00 | 60.80 |
| | 3095 | CD | PRO | 332 | 95.978 | 58.616 | 42.892 | 1.00 | 59.09 |
| | 3096 | N | ASP | 333 | 98.944 | 62.210 | 42.585 | 1.00 | 68.56 |
| | 3097 | CA | ASP | 333 | 100.324 | 62.554 | 42.237 | 1.00 | 71.37 |
| | 3098 | C | ASP | 333 | 101.432 | 61.520 | 42.437 | 1.00 | 68.42 |
| 40 | 3099 | O | ASP | 333 | 102.188 | 61.247 | 41.504 | 1.00 | 65.66 |
| | 3100 | CB | ASP | 333 | 100.715 | 63.879 | 42.891 | 1.00 | 79.84 |
| | 3101 | CG | ASP | 333 | 99.967 | 65.057 | 42.298 | 1.00 | 86.67 |
| | 3102 | OD1 | ASP | 333 | 100.442 | 65.608 | 41.283 | 1.00 | 91.38 |
| | 3103 | OD2 | ASP | 333 | 98.897 | 65.418 | 42.834 | 1.00 | 90.77 |
| 45 | 3104 | H | ASP | 333 | 98.343 | 62.928 | 42.866 | 1.00 | 25.00 |
| | 3105 | N | TYR | 334 | 101.536 | 60.936 | 43.627 | 1.00 | 65.59 |
| | 3106 | CA | TYR | 334 | 102.588 | 59.953 | 43.861 | 1.00 | 63.25 |
| | 3107 | C | TYR | 334 | 102.455 | 58.740 | 42.938 | 1.00 | 60.61 |
| | 3108 | O | TYR | 334 | 103.452 | 58.243 | 42.411 | 1.00 | 63.00 |
| 50 | 3109 | CB | TYR | 334 | 102.664 | 59.545 | 45.341 | 1.00 | 65.74 |
| | 3110 | CG | TYR | 334 | 101.539 | 58.674 | 45.852 | 1.00 | 68.46 |
| | 3111 | CD1 | TYR | 334 | 100.343 | 59.232 | 46.303 | 1.00 | 69.57 |

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|----|------|-----|-----|------|---------|--------|--------|------|-------|
| | 3112 | CD2 | TYR | 334 | 101.690 | 57.289 | 45.929 | 1.00 | 68.64 |
| | 3113 | CE1 | TYR | 334 | 99.326 | 58.432 | 46.824 | 1.00 | 69.54 |
| | 3114 | CE2 | TYR | 334 | 100.682 | 56.482 | 46.446 | 1.00 | 69.64 |
| | 3115 | CZ | TYR | 334 | 99.504 | 57.058 | 46.892 | 1.00 | 70.47 |
| 5 | 3116 | OH | TYR | 334 | 98.515 | 56.257 | 47.413 | 1.00 | 68.60 |
| | 3117 | H | TYR | 334 | 100.910 | 61.170 | 44.337 | 1.00 | 25.00 |
| | 3118 | HH | TYR | 334 | 97.786 | 56.812 | 47.691 | 1.00 | 25.00 |
| | 3119 | N | MET | 335 | 101.220 | 58.311 | 42.691 | 1.00 | 51.84 |
| | 3120 | CA | MET | 335 | 100.977 | 57.174 | 41.809 | 1.00 | 46.91 |
| 10 | 3121 | C | MET | 335 | 101.236 | 57.558 | 40.356 | 1.00 | 46.00 |
| | 3122 | O | MET | 335 | 101.540 | 56.701 | 39.525 | 1.00 | 49.65 |
| | 3123 | CB | MET | 335 | 99.552 | 56.646 | 41.969 | 1.00 | 41.83 |
| | 3124 | CG | MET | 335 | 99.268 | 56.054 | 43.333 | 1.00 | 37.39 |
| | 3125 | SD | MET | 335 | 97.625 | 55.322 | 43.450 | 1.00 | 44.89 |
| 15 | 3126 | CE | MET | 335 | 97.914 | 54.042 | 44.666 | 1.00 | 45.77 |
| | 3127 | H | MET | 335 | 100.460 | 58.772 | 43.094 | 1.00 | 25.00 |
| | 3128 | N | LYS | 336 | 101.122 | 58.848 | 40.052 | 1.00 | 47.61 |
| | 3129 | CA | LYS | 336 | 101.366 | 59.340 | 38.699 | 1.00 | 48.27 |
| | 3130 | C | LYS | 336 | 102.836 | 59.143 | 38.325 | 1.00 | 46.89 |
| 20 | 3131 | O | LYS | 336 | 103.161 | 58.829 | 37.177 | 1.00 | 49.33 |
| | 3132 | CB | LYS | 336 | 101.000 | 60.824 | 38.588 | 1.00 | 51.58 |
| | 3133 | CG | LYS | 336 | 99.517 | 61.132 | 38.743 | 1.00 | 54.94 |
| | 3134 | CD | LYS | 336 | 99.233 | 62.600 | 38.446 | 1.00 | 60.67 |
| | 3135 | CE | LYS | 336 | 97.739 | 62.882 | 38.431 | 1.00 | 63.81 |
| 25 | 3136 | NZ | LYS | 336 | 97.404 | 64.287 | 38.083 | 1.00 | 68.16 |
| | 3137 | H | LYS | 336 | 100.869 | 59.485 | 40.750 | 1.00 | 25.00 |
| | 3138 | 1HZ | LYS | 336 | 97.836 | 64.931 | 38.776 | 1.00 | 25.00 |
| | 3139 | 2HZ | LYS | 336 | 97.770 | 64.503 | 37.134 | 1.00 | 25.00 |
| | 3140 | 3HZ | LYS | 336 | 96.371 | 64.409 | 38.092 | 1.00 | 25.00 |
| 30 | 3141 | N | ILE | 337 | 103.719 | 59.321 | 39.303 | 1.00 | 44.56 |
| | 3142 | CA | ILE | 337 | 105.154 | 59.162 | 39.089 | 1.00 | 47.99 |
| | 3143 | C | ILE | 337 | 105.469 | 57.701 | 38.782 | 1.00 | 50.21 |
| | 3144 | O | ILE | 3337 | 106.153 | 57.400 | 37.800 | 1.00 | 52.97 |
| | 3145 | CB | ILE | 337 | 105.957 | 59.595 | 40.336 | 1.00 | 51.57 |
| 35 | 3146 | CG1 | ILE | 337 | 105.533 | 61.001 | 40.770 | 1.00 | 54.20 |
| | 3147 | CG2 | ILE | 337 | 107.455 | 59.569 | 40.034 | 1.00 | 49.66 |
| | 3148 | CD1 | ILE | 337 | 106.048 | 61.406 | 42.131 | 1.00 | 53.35 |
| | 3149 | H | ILE | 337 | 103.390 | 59.566 | 40.195 | 1.00 | 25.00 |
| | 3150 | N | SER | 338 | 104.951 | 56.802 | 39.618 | 1.00 | 46.40 |
| 40 | 3151 | CA | SER | 338 | 105.161 | 55.364 | 39.458 | 1.00 | 41.92 |
| | 3152 | C | SER | 338 | 104.640 | 54.905 | 38.098 | 1.00 | 39.82 |
| | 3153 | O | SER | 338 | 105.385 | 54.347 | 37.286 | 1.00 | 36.78 |
| | 3154 | CB | SER | 338 | 104.423 | 54.598 | 40.560 | 1.00 | 37.35 |
| | 3155 | OG | SER | 338 | 104.502 | 55.268 | 41.805 | 1.00 | 52.45 |
| 45 | 3156 | H | SER | 338 | 104.411 | 57.109 | 40.381 | 1.00 | 25.00 |
| | 3157 | HG | SER | 338 | 105.419 | 55.324 | 42.084 | 1.00 | 25.00 |
| | 3158 | N | TYR | 339 | 103.363 | 55.183 | 37.848 | 1.00 | 39.53 |
| | 3159 | CA | TYR | 339 | 102.697 | 54.804 | 36.606 | 1.00 | 40.68 |
| | 3160 | C | TYR | 339 | 103.468 | 55.247 | 35.362 | 1.00 | 39.79 |
| 50 | 3161 | O | TYR | 339 | 103.719 | 54.444 | 34.458 | 1.00 | 39.78 |
| | 3162 | CB | TYR | 339 | 101.272 | 55.374 | 36.586 | 1.00 | 39.96 |
| | 3163 | CG | TYR | 339 | 100.388 | 54.833 | 35.480 | 1.00 | 44.71 |

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|----|------|-----|-----|-----|---------|---------|--------|------|-------|
| | 3164 | CD1 | TYR | 339 | 99.948 | 53.507 | 35.494 | 1.00 | 40.18 |
| | 3165 | CD2 | TYR | 339 | 99.992 | 55.646 | 34.416 | 1.00 | 42.64 |
| | 3166 | CE1 | TYR | 339 | 99.136 | 53.004 | 34.475 | 1.00 | 40.02 |
| | 3167 | CE2 | TYR | 339 | 99.180 | 55.151 | 33.393 | 1.00 | 46.52 |
| 5 | 3168 | CZ | TYR | 339 | 98.758 | 53.830 | 33.431 | 1.00 | 40.74 |
| | 3169 | OH | TYR | 339 | 97.968 | 53.3422 | 32.417 | 1.00 | 44.28 |
| | 3170 | H | TYR | 339 | 102.843 | 55.668 | 38.522 | 1.00 | 25.00 |
| | 3171 | HH | TYR | 339 | 97.819 | 54.042 | 31.792 | 1.00 | 25.00 |
| | 3172 | N | LYS | 340 | 103.864 | 56.515 | 35.324 | 1.00 | 42.19 |
| 10 | 3173 | CA | LYS | 340 | 104.599 | 57.032 | 34.179 | 1.00 | 42.37 |
| | 3174 | C | LYS | 340 | 105.930 | 56.306 | 33.992 | 1.00 | 40.71 |
| | 3175 | O | LYS | 340 | 106.264 | 55.885 | 32.882 | 1.00 | 41.93 |
| | 3176 | CB | LYS | 340 | 104.826 | 58.541 | 34.306 | 1.00 | 48.48 |
| | 3177 | CG | LYS | 340 | 105.461 | 59.136 | 33.063 | 1.00 | 61.36 |
| 15 | 3178 | CD | LYS | 340 | 105.412 | 60.647 | 33.041 | 1.00 | 76.14 |
| | 3179 | CE | LYS | 340 | 105.947 | 61.164 | 31.713 | 1.00 | 85.02 |
| | 3180 | NZ | LYS | 340 | 105.783 | 62.636 | 31.566 | 1.00 | 94.84 |
| | 3181 | H | LYS | 340 | 103.661 | 57.115 | 36.074 | 1.00 | 25.00 |
| | 3182 | 1HZ | LYS | 340 | 104.774 | 62.881 | 31.624 | 1.00 | 25.00 |
| 20 | 3183 | 2HZ | LYS | 340 | 106.302 | 63.119 | 32.327 | 1.00 | 25.00 |
| | 3184 | 3HZ | LYS | 340 | 106.160 | 62.937 | 30.645 | 1.00 | 25.00 |
| | 3185 | N | ALA | 341 | 106.668 | 56.134 | 35.084 | 1.00 | 40.84 |
| | 3186 | CA | ALA | 341 | 107.963 | 55.455 | 35.052 | 1.00 | 36.82 |
| | 3187 | C | ALA | 341 | 107.837 | 54.053 | 34.469 | 1.00 | 35.10 |
| 25 | 3188 | O | ALA | 341 | 108.657 | 53.635 | 33.650 | 1.00 | 34.92 |
| | 3189 | CB | ALA | 341 | 108.548 | 55.388 | 36.451 | 1.00 | 37.09 |
| | 3190 | H | ALA | 341 | 106.336 | 56.478 | 35.942 | 1.00 | 25.00 |
| | 3191 | N | ILE | 342 | 106.796 | 53.338 | 34.884 | 1.00 | 32.81 |
| | 3192 | CA | ILE | 342 | 106.547 | 51.983 | 34.409 | 1.00 | 31.78 |
| 30 | 3193 | C | ILE | 342 | 106.357 | 51.982 | 32.891 | 1.00 | 38.13 |
| | 3194 | O | ILE | 342 | 107.061 | 51.269 | 32.163 | 1.00 | 37.84 |
| | 3195 | CB | ILE | 342 | 105.306 | 51.377 | 35.109 | 1.00 | 27.44 |
| | 3196 | CG1 | ILE | 342 | 105.585 | 51.219 | 36.606 | 1.00 | 30.45 |
| | 3197 | CG2 | ILE | 342 | 104.943 | 50.031 | 34.499 | 1.00 | 29.34 |
| 35 | 3198 | CD1 | ILE | 342 | 104.399 | 50.759 | 37.420 | 1.00 | 30.40 |
| | 3199 | H | ILE | 342 | 106.179 | 53.740 | 35.532 | 1.00 | 25.00 |
| | 3200 | N | LEU | 343 | 105.447 | 52.827 | 32.414 | 1.00 | 44.76 |
| | 3201 | CA | LEU | 343 | 105.168 | 52.920 | 30.984 | 1.00 | 42.79 |
| | 3202 | C | LEU | 343 | 106.428 | 53.290 | 30.214 | 1.00 | 40.23 |
| 40 | 3203 | O | LEU | 343 | 106.706 | 52.724 | 29.153 | 1.00 | 39.11 |
| | 3204 | CB | LEU | 343 | 104.061 | 53.943 | 30.715 | 1.00 | 42.96 |
| | 3205 | CG | LEU | 343 | 102.731 | 53.704 | 31.436 | 1.00 | 46.89 |
| | 3206 | CD1 | LEU | 343 | 101.704 | 54.723 | 30.978 | 1.00 | 51.34 |
| | 3207 | CD2 | LEU | 343 | 102.233 | 52.302 | 31.166 | 1.00 | 44.17 |
| 45 | 3208 | H | LEU | 343 | 104.954 | 53.403 | 33.039 | 1.00 | 25.00 |
| | 3209 | N | ASP | 344 | 107.202 | 54.218 | 30.770 | 1.00 | 40.93 |
| | 3210 | CA | ASP | 344 | 108.442 | 54.660 | 30.144 | 1.00 | 43.89 |
| | 3211 | C | ASP | 344 | 109.443 | 53.515 | 30.053 | 1.00 | 43.08 |
| | 3212 | O | ASP | 344 | 110.049 | 53.299 | 29.001 | 1.00 | 38.31 |
| 50 | 3213 | CB | ASP | 344 | 109.056 | 55.831 | 30.921 | 1.00 | 50.27 |
| | 3214 | CG | ASP | 344 | 108.259 | 57.124 | 30.775 | 1.00 | 58.66 |
| | 3215 | OD1 | ASP | 344 | 107.376 | 57.206 | 29.891 | 1.00 | 59.02 |

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|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 3216 | OD2 | ASP | 344 | 108.525 | 58.070 | 31.549 | 1.00 | 62.70 |
| | 3217 | H | ASP | 344 | 106.928 | 54.612 | 31.623 | 1.00 | 25.00 |
| | 3218 | N | LEU | 345 | 109.585 | 52.764 | 31.144 | 1.00 | 40.54 |
| | 3219 | CA | LEU | 345 | 110.511 | 51.633 | 31.196 | 1.00 | 36.66 |
| 5 | 3220 | C | LEU | 345 | 110.256 | 50.661 | 30.048 | 1.00 | 36.17 |
| | 3221 | O | LEU | 345 | 111.188 | 50.256 | 29.343 | 1.00 | 35.58 |
| | 3222 | CB | LEU | 345 | 110.393 | 50.903 | 32.540 | 1.00 | 38.27 |
| | 3223 | CG | LEU | 345 | 111.284 | 49.672 | 32.755 | 1.00 | 35.02 |
| | 3224 | CD1 | LEU | 345 | 112.750 | 50.043 | 32.587 | 1.00 | 28.76 |
| 10 | 3225 | CD2 | LEU | 345 | 111.030 | 49.087 | 34.132 | 1.00 | 30.95 |
| | 3226 | H | LEU | 345 | 109.050 | 52.975 | 31.934 | 1.00 | 25.00 |
| | 3227 | N | TYR | 346 | 108.992 | 50.304 | 29.844 | 1.00 | 35.43 |
| | 3228 | CA | TYR | 346 | 108.650 | 49.389 | 28.768 | 1.00 | 32.38 |
| | 3229 | C | TYR | 346 | 108.906 | 49.969 | 27.388 | 1.00 | 34.86 |
| 15 | 3230 | O | TYR | 346 | 109.183 | 49.228 | 26.446 | 1.00 | 36.74 |
| | 3231 | CB | TYR | 346 | 107.227 | 48.870 | 28.927 | 1.00 | 33.82 |
| | 3232 | CG | TYR | 346 | 107.173 | 47.798 | 29.980 | 1.00 | 31.79 |
| | 3233 | CD1 | TYR | 346 | 107.531 | 46.487 | 29.675 | 1.00 | 34.43 |
| | 3234 | CD2 | TYR | 346 | 106.856 | 48.107 | 31.302 | 1.00 | 34.30 |
| 20 | 3235 | CE1 | TYR | 346 | 107.585 | 45.507 | 30.659 | 1.00 | 32.57 |
| | 3236 | CE2 | TYR | 346 | 106.906 | 47.137 | 32.296 | 1.00 | 34.14 |
| | 3237 | CZ | TYR | 346 | 107.275 | 45.839 | 31.965 | 1.00 | 34.31 |
| | 3238 | OH | TYR | 346 | 107.351 | 44.878 | 32.938 | 1.00 | 32.03 |
| | 3239 | H | TYR | 346 | 108.288 | 50.665 | 30.428 | 1.00 | 25.00 |
| 25 | 3240 | HH | TYR | 346 | 107.610 | 44.036 | 32.562 | 1.00 | 25.00 |
| | 3241 | N | LYS | 347 | 108.861 | 51.295 | 27.276 | 1.00 | 44.24 |
| | 3242 | CA | LYS | 347 | 109.143 | 51.955 | 26.004 | 1.00 | 44.41 |
| | 3243 | C | LYS | 347 | 110.630 | 51.792 | 25.716 | 1.00 | 43.81 |
| | 3244 | O | LYS | 347 | 111.030 | 51.558 | 24.572 | 1.00 | 42.39 |
| 30 | 3245 | CB | LYS | 347 | 108.762 | 53.437 | 26.060 | 1.00 | 51.50 |
| | 3246 | CG | LYS | 347 | 107.268 | 53.672 | 25.945 | 1.00 | 55.25 |
| | 3247 | CD | LYS | 347 | 106.759 | 53.062 | 24.650 | 1.00 | 59.99 |
| | 3248 | CE | LYS | 347 | 105.251 | 52.978 | 24.608 | 1.00 | 60.17 |
| | 3249 | NZ | LYS | 347 | 104.841 | 52.152 | 23.446 | 1.00 | 53.42 |
| 35 | 3250 | H | LYS | 347 | 108.627 | 51.840 | 28.057 | 1.00 | 25.00 |
| | 3251 | 1HZ | LYS | 347 | 105.241 | 51.196 | 23.537 | 1.00 | 25.00 |
| | 3252 | 2HZ | LYS | 347 | 103.803 | 52.090 | 23.409 | 1.00 | 25.00 |
| | 3253 | 3HZ | LYS | 347 | 105.190 | 52.590 | 22.569 | 1.00 | 25.00 |
| | 3254 | N | ASP | 348 | 111.439 | 51.874 | 26.771 | 1.00 | 45.04 |
| 40 | 3255 | CA | ASP | 348 | 112.884 | 51.712 | 26.654 | 1.00 | 47.19 |
| | 3256 | C | ASP | 348 | 113.178 | 50.289 | 26.211 | 1.00 | 44.53 |
| | 3257 | O | ASP | 348 | 113.992 | 50.074 | 25.316 | 1.00 | 46.94 |
| | 3258 | CB | ASP | 348 | 113.582 | 51.981 | 27.991 | 1.00 | 55.77 |
| | 3259 | CG | ASP | 348 | 113.469 | 53.430 | 28.441 | 1.00 | 63.79 |
| 45 | 3260 | OD1 | ASP | 348 | 113.017 | 54.288 | 27.648 | 1.00 | 66.77 |
| | 3261 | OD2 | ASP | 348 | 113.846 | 53.710 | 29.600 | 1.00 | 65.20 |
| | 3262 | H | ASP | 348 | 111.048 | 52.057 | 27.652 | 1.00 | 25.00 |
| | 3263 | N | TYR | 349 | 112.507 | 49.321 | 26.835 | 1.00 | 39.87 |
| | 3264 | CA | TYR | 349 | 112.692 | 47.913 | 26.491 | 1.00 | 40.93 |
| 50 | 3265 | C | TYR | 349 | 112.412 | 47.704 | 25.008 | 1.00 | 41.26 |
| | 3266 | O | TYR | 349 | 113.189 | 47.051 | 24.302 | 1.00 | 40.44 |
| | 3267 | CB | TYR | 349 | 111.752 | 47.015 | 27.310 | 1.00 | 35.88 |

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|----|------|-----|------|-----|---------|--------|--------|------|-------|
| | 3268 | CG | TYR | 349 | 112.115 | 46.841 | 28.773 | 1.00 | 33.98 |
| | 3269 | CD1 | TYR | 349 | 113.396 | 47.144 | 29.250 | 1.00 | 29.99 |
| | 3270 | CD2 | TYR | 349 | 111.172 | 46.360 | 29.680 | 1.00 | 27.01 |
| 5 | 3271 | CE1 | TYR | 349 | 113.723 | 46.971 | 30.596 | 1.00 | 27.43 |
| | 3272 | CE2 | TYR | 349 | 111.485 | 46.182 | 31.021 | 1.00 | 32.24 |
| | 3273 | CZ | TYR | 349 | 112.759 | 46.491 | 31.476 | 1.00 | 34.71 |
| | 3274 | OH | TYR | 349 | 113.045 | 46.346 | 32.813 | 1.00 | 31.76 |
| | 3275 | H | TYR | 349 | 111.880 | 49.567 | 27.549 | 1.00 | 25.00 |
| | 3276 | HH | TYR | 349 | 112.295 | 45.961 | 33.270 | 1.00 | 25.00 |
| 10 | 3277 | N | GLU | 350 | 111.302 | 48.269 | 24.541 | 1.00 | 44.18 |
| | 3278 | CA | GLU | 350 | 110.911 | 48.156 | 23.140 | 1.00 | 47.18 |
| | 3279 | C | GLU | 350 | 111.972 | 48.767 | 22.235 | 1.00 | 45.46 |
| | 3280 | O | GLU | 350 | 112.337 | 48.175 | 21.221 | 1.00 | 45.14 |
| | 3281 | CB | GLU | 350 | 109.557 | 48.828 | 22.903 | 1.00 | 48.54 |
| 15 | 3282 | CG | GLU | 350 | 108.396 | 48.141 | 23.609 | 1.00 | 52.79 |
| | 3283 | CD | GLLU | 350 | 107.076 | 48.883 | 23.473 | 1.00 | 59.87 |
| | 3284 | OE1 | GLU | 350 | 107.070 | 50.040 | 23.000 | 1.00 | 66.09 |
| | 3285 | OE2 | GLU | 350 | 106.037 | 48.304 | 23.852 | 1.00 | 65.68 |
| | 3286 | H | GLU | 350 | 110.728 | 48.772 | 25.158 | 1.00 | 25.00 |
| 20 | 3287 | N | LYS | 351 | 112.497 | 49.923 | 22.636 | 1.00 | 48.01 |
| | 3288 | CA | LYS | 351 | 113.530 | 50.618 | 21.871 | 1.00 | 51.81 |
| | 3289 | C | LYS | 351 | 114.794 | 49.756 | 21.788 | 1.00 | 52.11 |
| | 3290 | O | LYS | 351 | 115.311 | 49.505 | 20.696 | 1.00 | 48.04 |
| | 3291 | CB | LYS | 351 | 113.861 | 51.973 | 22.518 | 1.00 | 53.86 |
| 25 | 3292 | CG | LYS | 351 | 114.151 | 53.095 | 21.520 | 1.00 | 60.98 |
| | 3293 | CD | LYS | 351 | 115.235 | 52.708 | 20.517 | 1.00 | 68.26 |
| | 3294 | CE | LYS | 351 | 115.153 | 53.551 | 19.253 | 1.00 | 75.67 |
| | 3295 | NZ | LYS | 351 | 115.951 | 52.975 | 18.132 | 1.00 | 74.32 |
| | 3296 | H | LYS | 351 | 112.180 | 50.322 | 23.471 | 1.00 | 25.00 |
| 30 | 3297 | 1HZ | LYS | 351 | 116.950 | 52.914 | 18.410 | 1.00 | 25.00 |
| | 3298 | 2HZ | LYS | 351 | 115.590 | 52.025 | 17.907 | 1.00 | 25.00 |
| | 3299 | 3HZ | LYS | 351 | 115.855 | 53.584 | 17.293 | 1.00 | 25.00 |
| | 3300 | N | GLU | 352 | 115.275 | 49.297 | 22.944 | 1.00 | 56.12 |
| | 3301 | CA | GLU | 352 | 116.474 | 48.461 | 23.031 | 1.00 | 54.04 |
| 35 | 3302 | C | GLU | 352 | 116.409 | 47.241 | 22.120 | 1.00 | 52.28 |
| | 3303 | O | GLU | 352 | 117.410 | 46.851 | 21.514 | 1.00 | 52.78 |
| | 3304 | CB | GLU | 352 | 116.688 | 47.971 | 24.466 | 1.00 | 58.92 |
| | 3305 | CG | GLU | 352 | 117.135 | 49.023 | 25.460 | 1.00 | 67.31 |
| | 3306 | CD | GLU | 352 | 117.386 | 48.438 | 26.842 | 1.00 | 71.98 |
| 40 | 3307 | OE1 | GLU | 352 | 118.383 | 47.694 | 27.004 | 1.00 | 69.15 |
| | 3308 | OE2 | GLU | 352 | 116.582 | 48.718 | 27.760 | 1.00 | 65.74 |
| | 3309 | H | GLU | 352 | 114.800 | 49.527 | 23.762 | 1.00 | 25.00 |
| | 3310 | N | LEU | 353 | 115.235 | 46.624 | 22.052 | 1.00 | 49.88 |
| | 3311 | CA | LEU | 353 | 115.053 | 45.435 | 21.233 | 1.00 | 51.47 |
| 45 | 3312 | C | LEU | 353 | 114.701 | 45.732 | 19.772 | 1.00 | 55.82 |
| | 3313 | O | LEU | 353 | 114.606 | 44.809 | 18.955 | 1.00 | 56.53 |
| | 3314 | CB | LEU | 353 | 114.009 | 44.511 | 21.876 | 1.00 | 44.77 |
| | 3315 | CG | LEU | 353 | 114.320 | 44.017 | 23.297 | 1.00 | 40.31 |
| | 3316 | CD1 | LEU | 353 | 113.151 | 43.224 | 23.855 | 1.00 | 35.62 |
| 50 | 3317 | CD2 | LEU | 353 | 115.586 | 43.172 | 23.302 | 1.00 | 33.71 |
| | 3318 | H | LEU | 353 | 114.478 | 46.975 | 22.571 | 1.00 | 25.00 |
| | 3319 | N | SER | 354 | 114.538 | 47.012 | 19.437 | 1.00 | 62.13 |

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|----|-------|------|-----|-----|---------|--------|---------|------|-------|
| | 3320 | CA | SER | 354 | 114.202 | 47.423 | 18.071 | 1.00 | 66.31 |
| | 33221 | C | SER | 354 | 115.245 | 46.970 | 17.058 | 1.00 | 64.64 |
| | 3322 | O | SER | 354 | 114.904 | 46.378 | 16.035 | 1.00 | 66.26 |
| | 3323 | CB | SER | 354 | 114.043 | 48.945 | 17.978 | 1.00 | 69.09 |
| 5 | 3324 | OG | SER | 354 | 112.959 | 49.406 | 18.763 | 1.00 | 80.83 |
| | 3325 | H | SER | 354 | 114.623 | 47.710 | 20.121 | 1.00 | 25.00 |
| | 3326 | HG | SER | 354 | 112.888 | 50.360 | 18.684 | 1.00 | 25.00 |
| | 3327 | N | SER | 355 | 116.516 | 47.223 | 17.359 | 1.00 | 65.77 |
| | 3328 | CA | SER | 355 | 117.616 | 46.850 | 16.472 | 1.00 | 67.77 |
| 10 | 3329 | C | SER | 355 | 117.631 | 45.364 | 16.110 | 1.00 | 68.81 |
| | 3330 | O | SER | 355 | 118.082 | 44.990 | 15.028 | 1.00 | 69.36 |
| | 3331 | CB | SER | 355 | 118.956 | 47.245 | 17.099 | 1.00 | 66.08 |
| | 3332 | OG | SER | 355 | 119.067 | 46.741 | 18.419 | 1.00 | 68.44 |
| | 3333 | H | SER | 355 | 116.729 | 47.670 | 18.209 | 1.00 | 25.00 |
| 15 | 3334 | HG | SER | 355 | 119.043 | 45.780 | 18.416 | 1.00 | 25.00 |
| | 3335 | N | ALA | 356 | 117.150 | 44.525 | 17.024 | 1.00 | 69.39 |
| | 3336 | CA | ALA | 356 | 117.115 | 43.082 | 16.802 | 1.00 | 68.66 |
| | 3337 | C | ALA | 356 | 115.741 | 42.585 | 16.347 | 1.00 | 69.25 |
| | 3338 | O | ALA | 356 | 115.561 | 41.395 | 16.084 | 1.00 | 71.52 |
| 20 | 3339 | CB | ALA | 356 | 117.549 | 42.347 | 18.067 | 1.00 | 64.46 |
| | 3340 | H | ALA | 356 | 116.806 | 44.884 | 17.867 | 1.00 | 25.00 |
| | 3341 | N | GLY | 357 | 114.773 | 43.493 | 16.270 | 1.00 | 67.77 |
| | 3342 | CA | GLY | 357 | 113.432 | 43.118 | 15.854 | 1.00 | 62.16 |
| | 3343 | C | GLY | 357 | 112.754 | 42.202 | 16.856 | 1.00 | 58.02 |
| 25 | 3344 | O | GLY | 357 | 111.969 | 41.327 | 16.481 | 1.00 | 58.07 |
| | 3345 | H | GLY | 357 | 114.965 | 44.428 | 16.477 | 1.00 | 25.00 |
| | 3346 | N | ARG | 358 | 113.039 | 42.416 | 18.138 | 1.00 | 53.28 |
| | 3347 | CA | ARG | 358 | 112.461 | 41.601 | 19.204 | 1.00 | 50.96 |
| | 3348 | C | ARG | 358 | 111.486 | 42.359 | 20.106 | 1.00 | 50.55 |
| 30 | 3349 | O | ARG | 358 | 110.885 | 41.774 | 20.999 | 1.00 | 51.85 |
| | 3350 | CB | ARG | 358 | 113.568 | 40.953 | 20.047 | 1.00 | 44.69 |
| | 3351 | CG | ARG | 358 | 114.360 | 39.872 | 19.314 | 1.00 | 43.66 |
| | 3352 | CD | ARG | 358 | 115.389 | 39.206 | 20.217 | 1.00 | 43.11 |
| | 3353 | NE | ARG | 358 | 114.768 | 38.503 | 21.338 | 1.00 | 42.40 |
| 35 | 3354 | CZ | ARG | 358 | 114.997 | 38.783 | 22.618 | 1.00 | 43.84 |
| | 3355 | NH1 | ARG | 358 | 115.836 | 39.754 | 22.951 | 1.00 | 49.95 |
| | 3356 | NH2 | ARG | 358 | 114.389 | 38.089 | 23.571 | 1.00 | 45.03 |
| | 3357 | H | ARG | 358 | 113.664 | 43.136 | 18.368 | 1.00 | 25.00 |
| | 3358 | HE | ARG | 358 | 114.142 | 37.776 | 21.138 | 1.00 | 25.00 |
| 40 | 3359 | 1HH1 | ARG | 358 | 116.301 | 40.282 | 22.241 | 1.00 | 25.00 |
| | 3360 | 2HH1 | ARG | 358 | 116.006 | 39.958 | 23.915 | 1.00 | 25.00 |
| | 3361 | 1HH2 | ARG | 358 | 113.755 | 37.355 | 23.327 | 1.00 | 25.00 |
| | 3362 | 2HH2 | ARG | 358 | 114.562 | 38.301 | 24.533 | 1.00 | 25.00 |
| | 3363 | N | SER | 359 | 111.270 | 43.639 | 19.826 | 1.00 | 50.59 |
| 45 | 3364 | CA | SER | 359 | 110.363 | 44.464 | 20.625 | 1.00 | 47.98 |
| | 3365 | C | SER | 359 | 108.948 | 43.888 | 20.767 | 1.00 | 48.46 |
| | 3366 | O | SER | 359 | 108.247 | 44.177 | 21.737 | 1.00 | 46.16 |
| | 3367 | CB | SER | 359 | 110.315 | 45.879 | 20.050 | 1.00 | 51.38 |
| | 3368 | OG | SER | 359 | 110.450 | 45.839 | 18.639 | 1.00 | 63.31 |
| 50 | 3369 | H | SER | 359 | 111.730 | 44.045 | 19.067 | 1.00 | 25.00 |
| | 3370 | HG | SER | 359 | 111.323 | 45.514 | 18.419 | 1.00 | 25.00 |
| | 3371 | N | HIS | 360 | 108.559 | 43.029 | 19.8829 | 1.00 | 46.52 |

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|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 3372 | CA | HIS | 360 | 107.234 | 42.401 | 19.837 | 1.00 | 47.05 |
| | 3373 | C | HIS | 360 | 106.998 | 41.398 | 20.974 | 1.00 | 48.80 |
| | 3374 | O | HIS | 360 | 105.893 | 40.871 | 21.124 | 1.00 | 46.79 |
| | 3375 | CB | HIS | 360 | 106.971 | 41.713 | 18.492 | 1.00 | 47.13 |
| 5 | 3376 | CG | HIS | 360 | 108.026 | 40.724 | 18.100 | 1.00 | 47.23 |
| | 3377 | ND1 | HIS | 360 | 107.885 | 39.365 | 18.289 | 1.00 | 50.30 |
| | 3378 | CD2 | HIS | 360 | 109.242 | 40.899 | 17.532 | 1.00 | 49.82 |
| | 3379 | CE1 | HIS | 360 | 108.969 | 38.746 | 17.855 | 1.00 | 47.18 |
| | 3380 | NE2 | HIS | 360 | 109.808 | 39.655 | 17.391 | 1.00 | 46.40 |
| 10 | 3381 | H | HIS | 360 | 109.183 | 42.837 | 19.111 | 1.00 | 25.00 |
| | 3382 | HD1 | HIS | 360 | 107.098 | 38.919 | 18.675 | 1.00 | 25.00 |
| | 3383 | HE2 | HIS | 360 | 110.702 | 39.494 | 16.992 | 1.00 | 25.00 |
| | 3384 | N | ILE | 361 | 108.042 | 41.098 | 21.741 | 1.00 | 47.17 |
| | 3385 | CA | ILE | 361 | 107.922 | 40.152 | 22.845 | 1.00 | 40.37 |
| 15 | 3386 | C | ILE | 361 | 107.657 | 40.850 | 24.175 | 1.00 | 35.93 |
| | 3387 | O | ILE | 361 | 107.118 | 40.240 | 25.103 | 1.00 | 41.86 |
| | 3388 | CB | ILE | 361 | 109.187 | 39.277 | 22.987 | 1.00 | 44.49 |
| | 3389 | CG1 | ILE | 361 | 110.392 | 40.152 | 23.346 | 1.00 | 39.20 |
| | 3390 | CG2 | ILE | 361 | 109.421 | 38.477 | 21.707 | 1.00 | 38.28 |
| 20 | 3391 | CD1 | ILE | 361 | 111.680 | 39.405 | 23.464 | 1.00 | 49.02 |
| | 3392 | H | ILE | 361 | 108.913 | 41.517 | 21.574 | 1.00 | 25.00 |
| | 3393 | N | VAL | 362 | 108.007 | 42.131 | 24.256 | 1.00 | 29.83 |
| | 3394 | CA | VAL | 362 | 107.818 | 42.911 | 25.478 | 1.00 | 28.00 |
| | 3395 | C | VAL | 362 | 106.396 | 42.815 | 26.041 | 1.00 | 32.52 |
| 25 | 3396 | O | VAL | 362 | 106.209 | 42.788 | 27.262 | 1.00 | 34.43 |
| | 3397 | CB | VAL | 362 | 108.203 | 44.401 | 25.259 | 1.00 | 30.93 |
| | 3398 | CG1 | VAL | 362 | 107.851 | 45.233 | 26.484 | 1.00 | 28.70 |
| | 3399 | CG2 | VAL | 362 | 109.699 | 44.524 | 24.952 | 1.00 | 22.99 |
| | 3400 | H | VAL | 362 | 108.395 | 42.568 | 23.472 | 1.00 | 25.00 |
| 30 | 3401 | N | CYS | 363 | 105.405 | 42.701 | 25.160 | 1.00 | 29.77 |
| | 3402 | CA | CYS | 363 | 104.011 | 42.610 | 25.592 | 1.00 | 31.29 |
| | 3403 | C | CYS | 363 | 103.757 | 41.470 | 26.581 | 1.00 | 29.63 |
| | 3404 | O | CYS | 363 | 102.942 | 41.610 | 27.499 | 1.00 | 25.93 |
| | 3405 | CB | CYS | 363 | 103.066 | 42.504 | 24.387 | 1.00 | 33.73 |
| 35 | 3406 | SG | CYS | 363 | 103.387 | 41.126 | 23.270 | 1.00 | 40.61 |
| | 3407 | H | CYS | 363 | 105.612 | 42.677 | 24.204 | 1.00 | 25.00 |
| | 3408 | N | HIS | 364 | 104.480 | 40.362 | 26.421 | 1.00 | 26.78 |
| | 3409 | CA | HIS | 364 | 104.332 | 39.216 | 27.315 | 1.00 | 24.36 |
| | 3410 | C | HIS | 364 | 104.685 | 39.599 | 28.754 | 1.00 | 31.26 |
| 40 | 3411 | O | HIS | 364 | 104.029 | 39.163 | 29.703 | 1.00 | 32.48 |
| | 3412 | CB | HIS | 364 | 105.220 | 38.064 | 26.855 | 1.00 | 26.25 |
| | 3413 | CG | HIS | 364 | 104.826 | 37.486 | 25.531 | 1.00 | 29.86 |
| | 3414 | ND1 | HIS | 364 | 103.731 | 36.663 | 25.372 | 1.00 | 39.99 |
| | 3415 | CD2 | HIS | 364 | 105.398 | 37.588 | 24.308 | 1.00 | 32.37 |
| 45 | 3416 | CE1 | HIS | 364 | 103.646 | 36.282 | 24.110 | 1.00 | 36.28 |
| | 3417 | NE2 | HIS | 364 | 104.646 | 36.829 | 23.444 | 1.00 | 32.87 |
| | 3418 | H | HIS | 364 | 105.139 | 40.332 | 25.695 | 1.00 | 25.00 |
| | 3419 | HD1 | HIS | 364 | 103.113 | 36.392 | 26.086 | 1.00 | 25.00 |
| | 3420 | HE2 | HIS | 364 | 104.819 | 36.718 | 22.488 | 1.00 | 25.00 |
| 50 | 3421 | N | ALA | 365 | 105.711 | 40.431 | 28.911 | 1.00 | 28.85 |
| | 3422 | CA | ALA | 365 | 106.134 | 40.880 | 30.232 | 1.00 | 30.11 |
| | 3423 | C | ALA | 365 | 105.075 | 41.813 | 30.826 | 1.00 | 31.00 |

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|----|------|------|-----|-----|---------|--------|--------|------|-------|
| | 3424 | O | ALA | 365 | 104.727 | 41.708 | 32.005 | 1.00 | 31.25 |
| | 3425 | CB | ALA | 365 | 107.482 | 41.585 | 30.140 | 1.00 | 31.82 |
| | 3426 | H | ALA | 365 | 106.191 | 40.762 | 28.123 | 1.00 | 25.00 |
| | 3427 | N | ILE | 366 | 104.548 | 42.708 | 29.992 | 1.00 | 33.54 |
| 5 | 3428 | CA | ILE | 366 | 103.512 | 43.653 | 30.417 | 1.00 | 33.21 |
| | 3429 | C | ILE | 366 | 102.287 | 42.889 | 30.922 | 1.00 | 29.56 |
| | 3430 | O | ILE | 366 | 101.743 | 43.199 | 31.987 | 1.00 | 31.04 |
| | 3431 | CB | ILE | 366 | 103.086 | 44.582 | 29.255 | 1.00 | 33.17 |
| | 3432 | CG1 | ILE | 366 | 104.264 | 45.455 | 28.823 | 1.00 | 30.87 |
| 10 | 3433 | CG2 | ILE | 366 | 101.908 | 45.453 | 29.674 | 1.00 | 28.96 |
| | 3434 | CD1 | ILE | 366 | 103.987 | 46.289 | 27.599 | 1.00 | 35.02 |
| | 3435 | H | ILE | 366 | 104.869 | 42.731 | 29.067 | 1.00 | 25.00 |
| | 3436 | N | GLU | 367 | 101.874 | 41.875 | 30.167 | 1.00 | 28.47 |
| | 3437 | CA | GLU | 367 | 100.726 | 41.061 | 30.548 | 1.00 | 30.13 |
| 15 | 3438 | C | GLU | 367 | 100.945 | 40.439 | 31.929 | 1.00 | 30.58 |
| | 3439 | O | GLU | 367 | 100.029 | 40.407 | 32.754 | 1.00 | 31.55 |
| | 3440 | CB | GLU | 367 | 100.461 | 39.966 | 29.507 | 1.00 | 38.78 |
| | 3441 | CG | GLU | 367 | 100.228 | 40.472 | 28.074 | 1.00 | 52.31 |
| | 3442 | CD | GLU | 367 | 99.180 | 41.585 | 27.970 | 1.00 | 62.83 |
| 20 | 3443 | OE1 | GLU | 367 | 98.144 | 41.525 | 28.675 | 1.00 | 55.58 |
| | 3444 | OE2 | GLU | 367 | 99.395 | 42.523 | 27.168 | 1.00 | 63.90 |
| | 3445 | H | GLU | 367 | 102.351 | 41.673 | 29.337 | 1.00 | 25.00 |
| | 3446 | N | ARG | 368 | 102.167 | 39.985 | 32.196 | 1.00 | 28.25 |
| | 3447 | CA | ARG | 368 | 102.479 | 39.385 | 33.487 | 1.00 | 21.98 |
| 25 | 3448 | C | ARG | 368 | 102.462 | 40.420 | 34.607 | 1.00 | 22.36 |
| | 3449 | O | ARG | 368 | 102.080 | 40.108 | 35.738 | 1.00 | 22.36 |
| | 3450 | CB | ARG | 368 | 103.821 | 38.661 | 33.440 | 1.00 | 23.96 |
| | 3451 | CG | ARG | 368 | 103.796 | 37.364 | 32.642 | 1.00 | 17.80 |
| | 3452 | CD | ARG | 368 | 102.812 | 36.352 | 33.224 | 1.00 | 19.62 |
| 30 | 3453 | NE | ARG | 368 | 103.008 | 35.034 | 32.626 | 1.00 | 19.60 |
| | 3454 | CZ | ARG | 368 | 102.516 | 33.897 | 33.113 | 1.00 | 20.41 |
| | 3455 | NH1 | ARG | 368 | 101.773 | 33.898 | 34.211 | 1.00 | 26.21 |
| | 3456 | NH2 | ARG | 368 | 102.843 | 32.743 | 32.548 | 1.00 | 22.02 |
| | 3457 | H | ARG | 368 | 102.868 | 40.046 | 31.510 | 1.00 | 25.00 |
| 35 | 3458 | HE | ARG | 368 | 103.526 | 34.993 | 31.804 | 1.00 | 25.00 |
| | 3459 | 1HH1 | ARG | 368 | 101.580 | 34.754 | 34.685 | 1.00 | 25.00 |
| | 3460 | 2HH1 | ARG | 368 | 101.410 | 33.036 | 34.566 | 1.00 | 25.00 |
| | 3461 | 1HH2 | ARG | 368 | 103.454 | 32.730 | 31.755 | 1.00 | 25.00 |
| | 3462 | 2HH2 | ARG | 368 | 102.476 | 31.888 | 32.904 | 1.00 | 25.00 |
| 40 | 3463 | N | MET | 369 | 102.849 | 41.654 | 34.293 | 1.00 | 23.19 |
| | 3464 | CA | MET | 369 | 102.845 | 42.716 | 35.295 | 1.00 | 20.55 |
| | 3465 | C | MET | 369 | 101.410 | 43.060 | 35.657 | 1.00 | 20.66 |
| | 3466 | O | MET | 369 | 101.085 | 43.248 | 36.833 | 1.00 | 24.28 |
| | 3467 | CB | MET | 369 | 103.565 | 43.966 | 34.789 | 1.00 | 24.43 |
| 45 | 3468 | CG | MET | 369 | 103.575 | 45.097 | 35.806 | 1.00 | 27.10 |
| | 3469 | SD | MET | 369 | 104.503 | 46.538 | 35.283 | 1.00 | 33.91 |
| | 3470 | CE | MET | 369 | 105.378 | 46.942 | 36.804 | 1.00 | 36.11 |
| | 3471 | H | MET | 369 | 103.151 | 41.852 | 33.380 | 1.00 | 25.00 |
| | 3472 | N | LYS | 370 | 100.550 | 43.142 | 34.645 | 1.00 | 27.52 |
| 50 | 3473 | CA | LYS | 370 | 99.135 | 43.441 | 34.865 | 1.00 | 27.03 |
| | 3474 | C | LYS | 370 | 98.572 | 42.392 | 35.817 | 1.00 | 26.80 |
| | 3475 | O | LYS | 370 | 97.854 | 42.720 | 36.766 | 1.00 | 31.01 |

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|----|------|------|-----|------|---------|---------|--------|------|-------|
| | 3476 | CB | LYS | 370 | 98.361 | 43.415 | 33.545 | 1.00 | 28.62 |
| | 3477 | CG | LYS | 370 | 98.699 | 44.546 | 32.591 | 1.00 | 26.77 |
| | 3478 | CD | LYS | 370 | 97.881 | 44.437 | 31.318 | 1.00 | 32.86 |
| | 3479 | CE | LYS | 370 | 98.174 | 45.591 | 30.371 | 1.00 | 40.98 |
| 5 | 3480 | NZ | LYS | 370 | 97.397 | 45.502 | 29.099 | 1.00 | 45.53 |
| | 3481 | H | LYS | 370 | 100.870 | 43.001 | 33.729 | 1.00 | 25.00 |
| | 3482 | 1HZ | LYS | 370 | 96.379 | 45.511 | 29.313 | 1.00 | 25.00 |
| | 3483 | 2HZ | LYS | 370 | 97.630 | 46.314 | 28.492 | 1.00 | 25.00 |
| | 3484 | 3HZ | LYS | 370 | 97.640 | 44.619 | 28.607 | 1.00 | 25.00 |
| 10 | 3485 | N | GLU | 3771 | 98.959 | 41.139 | 35.581 | 1.00 | 26.63 |
| | 3486 | CA | GLU | 371 | 98.541 | 40.006 | 36.398 | 1.00 | 23.18 |
| | 3487 | C | GLU | 371 | 98.981 | 40.191 | 37.854 | 1.00 | 31.56 |
| | 3488 | O | GLU | 371 | 98.180 | 40.023 | 38.782 | 1.00 | 33.30 |
| | 3489 | CB | GLU | 371 | 99.125 | 38.719 | 35.815 | 1.00 | 24.88 |
| 15 | 3490 | CG | GLU | 371 | 98.779 | 37.449 | 36.569 | 1.00 | 25.01 |
| | 3491 | CD | GLU | 371 | 99.346 | 36.212 | 35.892 | 1.00 | 38.13 |
| | 3492 | OE1 | GLU | 371 | 100.588 | 36.080 | 35.815 | 1.00 | 34.30 |
| | 3493 | OE2 | GLU | 371 | 98.549 | 35.373 | 35.425 | 1.00 | 44.97 |
| | 3494 | H | GLU | 371 | 99.542 | 40.972 | 34.811 | 1.00 | 25.00 |
| 20 | 3495 | N | VAL | 372 | 100.243 | 40.567 | 38.056 | 1.00 | 29.02 |
| | 3496 | CA | VAL | 372 | 100.765 | 40.789 | 39.406 | 1.00 | 26.07 |
| | 3497 | C | VAL | 372 | 99.952 | 41.869 | 40.126 | 1.00 | 28.22 |
| | 3498 | O | VAL | 372 | 99.582 | 41.705 | 41.293 | 1.00 | 27.36 |
| | 3499 | CB | VAL | 372 | 102.261 | 41.216 | 39.388 | 1.00 | 27.23 |
| 25 | 3500 | CG1 | VAL | 372 | 102.738 | 41.520 | 40.801 | 1.00 | 19.82 |
| | 3501 | CG2 | VAL | 372 | 103.124 | 40.119 | 38.770 | 1.00 | 23.40 |
| | 3502 | H | VAL | 372 | 100.836 | 40.688 | 37.283 | 1.00 | 25.00 |
| | 3503 | N | VAL | 373 | 99.657 | 42.964 | 39.426 | 1.00 | 31.06 |
| | 3504 | CA | VAL | 373 | 98.893 | 44.063 | 40.018 | 1.00 | 32.80 |
| 30 | 3505 | C | VAL | 373 | 97.453 | 43.670 | 40.378 | 1.00 | 33.82 |
| | 3506 | O | VAL | 373 | 96.952 | 44.054 | 41.441 | 1.00 | 30.74 |
| | 3507 | CB | VAL | 373 | 98.908 | 45.314 | 39.118 | 1.00 | 34.89 |
| | 3508 | CG1 | VAL | 373 | 98.134 | 46.454 | 39.775 | 1.00 | 32.71 |
| | 3509 | CG2 | VAL | 373 | 100.345 | 45.741 | 38.855 | 1.00 | 34.17 |
| 35 | 3510 | H | VAL | 373 | 99.960 | 43.0288 | 38.495 | 1.00 | 25.00 |
| | 3511 | N | ARG | 374 | 96.794 | 42.900 | 39.512 | 1.00 | 31.81 |
| | 3512 | CA | ARG | 374 | 95.428 | 42.447 | 39.789 | 1.00 | 29.59 |
| | 3513 | C | ARG | 374 | 95.422 | 41.667 | 41.093 | 1.00 | 31.35 |
| | 3514 | O | ARG | 374 | 94.613 | 41.933 | 41.989 | 1.00 | 36.45 |
| 40 | 3515 | CB | ARG | 374 | 94.910 | 41.519 | 38.689 | 1.00 | 29.25 |
| | 3516 | CG | ARG | 374 | 94.668 | 42.166 | 37.349 | 1.00 | 32.69 |
| | 3517 | CD | ARG | 374 | 94.034 | 41.169 | 36.396 | 1.00 | 33.05 |
| | 3518 | NE | ARG | 374 | 94.840 | 40.973 | 35.194 | 1.00 | 37.26 |
| | 3519 | CZ | ARG | 374 | 95.399 | 39.817 | 34.846 | 1.00 | 38.15 |
| 45 | 3520 | NH1 | ARG | 374 | 95.247 | 38.741 | 35.608 | 1.00 | 41.80 |
| | 3521 | NH2 | ARG | 374 | 96.114 | 39.738 | 33.733 | 1.00 | 40.61 |
| | 3522 | H | ARG | 374 | 97.230 | 42.625 | 38.677 | 1.00 | 25.00 |
| | 3523 | HE | ARG | 374 | 94.974 | 41.744 | 34.603 | 1.00 | 25.00 |
| | 3524 | 1HH1 | ARG | 374 | 94.711 | 38.795 | 36.448 | 1.00 | 25.00 |
| 50 | 3525 | 2HH1 | ARG | 374 | 95.672 | 37.878 | 35.336 | 1.00 | 25.00 |
| | 3526 | 1HH2 | ARG | 374 | 96.232 | 40.550 | 33.158 | 1.00 | 25.00 |
| | 3527 | 2HH2 | ARG | 374 | 96.537 | 38.873 | 33.467 | 1.00 | 25.00 |

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|----|------|------|-----|-----|---------|--------|--------|------|-------|
| | 3528 | N | ASN | 375 | 96.351 | 40.721 | 41.202 | 1.00 | 31.47 |
| | 3529 | CA | ASN | 375 | 96.458 | 39.883 | 42.388 | 1.00 | 28.79 |
| | 3530 | C | ASN | 375 | 96.897 | 40.652 | 43.625 | 1.00 | 26.40 |
| 5 | 3531 | O | ASN | 375 | 96.561 | 40.266 | 44.746 | 1.00 | 27.83 |
| | 3532 | CB | ASN | 375 | 97.359 | 38.683 | 42.112 | 1.00 | 35.49 |
| | 3533 | CG | ASN | 375 | 96.744 | 37.720 | 41.111 | 1.00 | 32.04 |
| | 3534 | OD1 | ASN | 375 | 95.982 | 38.125 | 40.237 | 1.00 | 33.82 |
| | 3535 | ND2 | ASN | 375 | 97.075 | 36.442 | 41.231 | 1.00 | 34.73 |
| 10 | 3536 | H | ASN | 375 | 96.970 | 40.566 | 40.454 | 1.00 | 25.00 |
| | 3537 | 1HD2 | ASN | 375 | 96.671 | 35.822 | 40.590 | 1.00 | 25.00 |
| | 3538 | 2HD2 | ASN | 375 | 97.686 | 36.184 | 41.941 | 1.00 | 25.00 |
| | 3539 | N | TYR | 376 | 97.643 | 41.736 | 43.422 | 1.00 | 32.41 |
| | 3540 | CA | TYR | 376 | 98.075 | 42.599 | 44.526 | 1.00 | 36.00 |
| 15 | 3541 | C | TYR | 376 | 96.803 | 43.220 | 45.101 | 1.00 | 36.51 |
| | 3542 | O | TYR | 376 | 96.585 | 43.247 | 46.316 | 1.00 | 32.23 |
| | 3543 | CB | TYR | 376 | 98.960 | 43.739 | 44.010 | 1.00 | 34.19 |
| | 3544 | CG | TYR | 376 | 100.447 | 43.464 | 43.979 | 1.00 | 41.46 |
| | 3545 | CD1 | TYR | 376 | 100.993 | 42.339 | 44.601 | 1.00 | 40.12 |
| | 3546 | CD2 | TYR | 376 | 101.315 | 44.350 | 43.336 | 1.00 | 41.43 |
| 20 | 3547 | CE1 | TYR | 376 | 102.365 | 42.104 | 44.580 | 1.00 | 38.75 |
| | 3548 | CE2 | TYR | 376 | 102.688 | 44.127 | 43.310 | 1.00 | 37.68 |
| | 3549 | CZ | TYR | 376 | 103.203 | 43.005 | 43.932 | 1.00 | 41.58 |
| | 3550 | OH | TYR | 376 | 104.560 | 42.785 | 43.895 | 1.00 | 43.07 |
| 25 | 3551 | H | TYR | 376 | 97.915 | 41.956 | 42.506 | 1.00 | 25.00 |
| | 3552 | HH | TYR | 376 | 104.761 | 41.958 | 44.341 | 1.00 | 25.00 |
| | 3553 | N | ASN | 377 | 95.965 | 43.713 | 44.194 | 1.00 | 37.58 |
| | 3554 | CA | ASN | 377 | 94.704 | 44.343 | 44.550 | 1.00 | 36.82 |
| | 3555 | C | ASN | 377 | 93.807 | 43.352 | 45.285 | 1.00 | 35.16 |
| | 3556 | O | ASN | 377 | 93.276 | 43.658 | 46.353 | 1.00 | 35.66 |
| 30 | 3557 | CB | ASN | 377 | 94.011 | 44.846 | 43.287 | 1.00 | 38.60 |
| | 3558 | CG | ASN | 377 | 92.858 | 45.770 | 43.587 | 1.00 | 43.38 |
| | 3559 | OD1 | ASN | 377 | 92.949 | 46.628 | 44.462 | 1.00 | 38.97 |
| | 3560 | ND2 | ASN | 377 | 91.774 | 45.622 | 42.838 | 1.00 | 46.57 |
| 35 | 3561 | H | ASN | 377 | 96.210 | 43.651 | 43.245 | 1.00 | 25.00 |
| | 3562 | 1HD2 | ASN | 377 | 91.023 | 46.218 | 43.029 | 1.00 | 25.00 |
| | 3563 | 2HD2 | ASN | 377 | 91.765 | 44.936 | 42.143 | 1.00 | 25.00 |
| | 3564 | N | VAL | 378 | 93.683 | 42.147 | 44.735 | 1.00 | 32.14 |
| | 3565 | CA | VAL | 378 | 92.857 | 41.106 | 45.344 | 1.00 | 28.96 |
| | 3566 | C | VAL | 378 | 93.339 | 40.801 | 46.766 | 1.00 | 33.76 |
| 40 | 3567 | O | VAL | 378 | 92.532 | 40.647 | 47.690 | 1.00 | 32.35 |
| | 3568 | CB | VAL | 378 | 92.858 | 39.818 | 44.490 | 1.00 | 30.20 |
| | 3569 | CG1 | VAL | 378 | 92.051 | 38.732 | 45.169 | 1.00 | 28.32 |
| | 3570 | CG2 | VAL | 378 | 92.285 | 40.104 | 43.105 | 1.00 | 26.65 |
| 45 | 3571 | H | VAL | 378 | 94.153 | 41.951 | 43.897 | 1.00 | 25.00 |
| | 3572 | N | GLU | 379 | 94.657 | 40.741 | 46.940 | 1.00 | 36.35 |
| | 3573 | CA | GLU | 379 | 95.258 | 40.478 | 48.246 | 1.00 | 38.43 |
| | 3574 | C | GLU | 379 | 94.875 | 41.598 | 49.209 | 1.00 | 36.80 |
| | 3575 | O | GLU | 379 | 94.579 | 41.352 | 50.383 | 1.00 | 37.49 |
| | 3576 | CB | GLU | 379 | 96.780 | 40.395 | 48.114 | 1.00 | 43.01 |
| 50 | 3577 | CG | GLU | 379 | 97.544 | 40.416 | 49.436 | 1.00 | 52.96 |
| | 3578 | CD | GLU | 379 | 99.055 | 40.403 | 49.250 | 1.00 | 61.44 |
| | 3579 | OE1 | GLU | 379 | 99.528 | 40.225 | 48.107 | 1.00 | 70.64 |

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|----|------|-----|------|-----|--------|--------|--------|------|-------|
| | 3580 | OE2 | GLU | 379 | 99.776 | 40.568 | 50.255 | 1.00 | 66.21 |
| | 3581 | H | GLU | 379 | 95.247 | 40.882 | 46.167 | 1.00 | 25.00 |
| | 3582 | N | SER | 380 | 94.894 | 42.827 | 48.700 | 1.00 | 37.49 |
| | 3583 | CA | SER | 380 | 94.531 | 44.003 | 49.480 | 1.00 | 38.42 |
| 5 | 3584 | C | SER | 380 | 93.070 | 43.865 | 49.906 | 1.00 | 37.35 |
| | 3585 | O | SER | 380 | 92.740 | 44.018 | 51.085 | 1.00 | 38.35 |
| | 3586 | CB | SER | 380 | 94.721 | 45.264 | 48.634 | 1.00 | 37.87 |
| | 3587 | OG | SER | 380 | 94.344 | 46.428 | 49.349 | 1.00 | 51.23 |
| | 3588 | H | SER | 380 | 95.167 | 42.951 | 47.767 | 1.00 | 25.00 |
| 10 | 3589 | HG | SER | 380 | 94.903 | 46.518 | 50.127 | 1.00 | 25.00 |
| | 3590 | N | THR | 381 | 92.209 | 43.535 | 48.945 | 1.00 | 36.73 |
| | 3591 | CA | THR | 381 | 90.785 | 43.349 | 49.198 | 1.00 | 31.81 |
| | 3592 | C | THR | 381 | 90.574 | 42.286 | 50.278 | 1.00 | 33.52 |
| | 3593 | O | THR | 381 | 89.846 | 42.514 | 51.245 | 1.00 | 35.95 |
| 15 | 3594 | CB | THR | 381 | 90.043 | 42.922 | 47.912 | 1.00 | 27.90 |
| | 3595 | OG1 | THR | 381 | 90.230 | 43.914 | 46.894 | 1.00 | 30.65 |
| | 3596 | CG2 | THR | 381 | 88.564 | 42.762 | 48.174 | 1.00 | 30.75 |
| | 3597 | H | THR | 381 | 92.531 | 43.424 | 48.030 | 1.00 | 25.00 |
| | 3598 | HG1 | THR | 381 | 89.901 | 44.765 | 47.202 | 1.00 | 25.00 |
| 20 | 3599 | N | TRP | 382 | 91.246 | 41.146 | 50.137 | 1.00 | 31.98 |
| | 3600 | CA | TRP | 382 | 91.124 | 40.059 | 51.106 | 1.00 | 34.10 |
| | 3601 | C | TRP | 382 | 91.498 | 40.511 | 52.513 | 1.00 | 37.61 |
| | 3602 | O | TRP | 382 | 90.840 | 40.145 | 53.490 | 1.00 | 37.71 |
| | 3603 | CB | TRP | 382 | 92.001 | 38.870 | 50.701 | 1.00 | 29.03 |
| 25 | 3604 | CG | TRP | 382 | 91.465 | 38.064 | 49.553 | 1.00 | 34.52 |
| | 3605 | CD1 | TRP | 382 | 90.298 | 38.272 | 48.872 | 1.00 | 32.13 |
| | 3606 | CD2 | TRP | 382 | 92.073 | 36.907 | 48.962 | 1.00 | 41.36 |
| | 3607 | NE1 | TRP | 382 | 90.141 | 37.315 | 47.897 | 1.00 | 33.27 |
| | 3608 | CE2 | TRP | 382 | 91.215 | 36.465 | 47.929 | 1.00 | 39.81 |
| 30 | 3609 | CE3 | TRP | 382 | 93.262 | 36.198 | 49.205 | 1.00 | 42.10 |
| | 3610 | CZ2 | TRP | 382 | 91.507 | 35.344 | 47.138 | 1.00 | 41.24 |
| | 3611 | CZ3 | TRP | 382 | 93.552 | 35.082 | 48.417 | 1.00 | 37.35 |
| | 3612 | CH2 | TRP | 382 | 92.676 | 34.669 | 47.396 | 1.00 | 37.45 |
| | 3613 | H | TRP | 382 | 91.841 | 41.035 | 49.370 | 1.00 | 25.00 |
| 35 | 3614 | HE1 | TRP | 382 | 89.384 | 37.250 | 47.275 | 1.00 | 25.00 |
| | 3615 | N | PHE | 383 | 92.551 | 41.317 | 52.601 | 1.00 | 42.79 |
| | 3616 | CA | PHE | 383 | 93.040 | 41.836 | 53.875 | 1.00 | 44.89 |
| | 3617 | C | PHE | 383 | 92.005 | 42.728 | 54.561 | 1.00 | 45.32 |
| | 3618 | O | PHE | 383 | 91.714 | 42.557 | 55.748 | 1.00 | 44.05 |
| 40 | 3619 | CB | PHE | 383 | 94.346 | 42.611 | 53.657 | 1.00 | 45.88 |
| | 3620 | CG | PHE | 383 | 94.818 | 43.358 | 54.869 | 1.00 | 46.79 |
| | 3621 | CD1 | PHE | 383 | 95.254 | 42.674 | 55.997 | 1.00 | 47.27 |
| | 3622 | CD2 | PHE | 383 | 94.800 | 44.751 | 54.893 | 1.00 | 50.35 |
| | 3623 | CE1 | PHE | 383 | 95.665 | 43.368 | 57.137 | 1.00 | 53.01 |
| 45 | 3624 | CE2 | PHHE | 383 | 95.208 | 45.453 | 56.026 | 1.00 | 50.27 |
| | 3625 | CZ | PHE | 383 | 95.641 | 44.759 | 57.151 | 1.00 | 48.55 |
| | 3626 | H | PHE | 383 | 93.023 | 41.569 | 51.778 | 1.00 | 25.00 |
| | 3627 | N | ILE | 384 | 91.462 | 43.677 | 53.803 | 1.00 | 46.83 |
| | 3628 | CA | ILE | 384 | 90.458 | 44.610 | 54.306 | 1.00 | 46.17 |
| 50 | 3629 | C | ILE | 384 | 89.185 | 43.894 | 54.774 | 1.00 | 47.27 |
| | 3630 | O | ILE | 384 | 88.608 | 44.253 | 55.799 | 1.00 | 47.11 |
| | 3631 | CB | ILE | 384 | 90.091 | 45.646 | 53.227 | 1.00 | 41.64 |

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|----|-------|-----|-----|-----|--------|--------|--------|------|-------|
| | 3632 | CG1 | ILE | 384 | 91.337 | 46.434 | 52.817 | 1.00 | 42.54 |
| | 3633 | CG2 | ILE | 384 | 89.031 | 46.597 | 53.750 | 1.00 | 46.00 |
| | 3634 | CD1 | ILE | 384 | 91.148 | 47.270 | 51.568 | 1.00 | 40.69 |
| | 3635 | H | ILE | 384 | 91.753 | 43.749 | 52.867 | 1.00 | 25.00 |
| 5 | 3636 | N | GLU | 385 | 88.756 | 42.884 | 54.022 | 1.00 | 45.25 |
| | 3637 | CA | GLU | 385 | 87.554 | 42.123 | 54.360 | 1.00 | 43.73 |
| | 3638 | C | GLU | 385 | 87.791 | 41.137 | 55.495 | 1.00 | 46.22 |
| | 3639 | O | GLU | 385 | 86.842 | 40.636 | 56.097 | 1.00 | 51.43 |
| | 3640 | CB | GLU | 385 | 87.051 | 41.346 | 53.142 | 1.00 | 42.68 |
| 10 | 3641 | CG | GLU | 385 | 86.657 | 42.211 | 51.956 | 1.00 | 46.85 |
| | 3642 | CD | GLU | 385 | 86.265 | 41.397 | 50.730 | 1.00 | 50.00 |
| | 3643 | OE1 | GLU | 385 | 86.535 | 40.175 | 50.696 | 1.00 | 44.05 |
| | 3644 | OE2 | GLU | 385 | 85.689 | 41.988 | 49.791 | 1.00 | 52.88 |
| | 3645 | H | GLU | 385 | 89.262 | 42.652 | 53.215 | 1.00 | 25.00 |
| 15 | 3646 | N | GLY | 386 | 89.055 | 40.846 | 55.777 | 1.00 | 45.48 |
| | 3647 | CA | GLY | 386 | 89.371 | 39.893 | 56.824 | 1.00 | 41.52 |
| | 3648 | C | GLY | 386 | 89.038 | 38.499 | 56.328 | 1.00 | 42.60 |
| | 3649 | O | GLY | 386 | 88.656 | 37.625 | 57.104 | 1.00 | 44.94 |
| | 3650 | H | GLY | 386 | 89.784 | 41.273 | 55.279 | 1.00 | 25.00 |
| 20 | 3651 | N | TYR | 387 | 89.190 | 38.297 | 55.023 | 1.00 | 42.34 |
| | 3652 | CA | TYR | 387 | 88.897 | 37.020 | 54.382 | 1.00 | 43.55 |
| | 3653 | C | TYR | 387 | 90.042 | 36.010 | 54.474 | 1.00 | 45.46 |
| | 3654 | O | TYR | 387 | 91.191 | 36.329 | 54.162 | 1.00 | 49.16 |
| | 3655 | CB | TYR | 387 | 88.545 | 37.254 | 52.908 | 1.00 | 38.26 |
| 25 | 3656 | CG | TYR | 387 | 88.082 | 36.017 | 52.162 | 1.00 | 36.21 |
| | 3657 | CD1 | TYR | 387 | 87.152 | 35.142 | 52.727 | 1.00 | 36.57 |
| | 3658 | CD2 | TYR | 387 | 88.555 | 35.736 | 50.880 | 1.00 | 31.64 |
| | 3659 | CE1 | TYR | 387 | 86.704 | 34.015 | 52.035 | 1.00 | 32.07 |
| | 3660 | CE2 | TYR | 387 | 88.112 | 34.616 | 50.178 | 1.00 | 32.41 |
| 30 | 3661 | CZ | TYR | 387 | 87.187 | 33.759 | 50.763 | 1.00 | 34.67 |
| | 36662 | OH | TYR | 387 | 86.749 | 32.646 | 50.082 | 1.00 | 38.16 |
| | 3663 | H | TYR | 387 | 89.541 | 39.025 | 54.474 | 1.00 | 25.00 |
| | 3664 | HH | TYR | 387 | 87.147 | 32.629 | 49.211 | 1.00 | 25.00 |
| | 3665 | N | THR | 388 | 89.706 | 34.787 | 54.872 | 1.00 | 45.36 |
| 35 | 3666 | CA | THR | 388 | 90.671 | 33.692 | 54.986 | 1.00 | 43.34 |
| | 3667 | C | THR | 388 | 90.199 | 32.571 | 54.048 | 1.00 | 41.02 |
| | 3668 | O | THR | 388 | 89.474 | 31.660 | 54.459 | 1.00 | 45.75 |
| | 3669 | CB | THR | 388 | 90.748 | 33.161 | 56.444 | 1.00 | 42.74 |
| | 3670 | OG1 | THR | 388 | 91.169 | 34.220 | 57.314 | 1.00 | 43.28 |
| 40 | 3671 | CG2 | THR | 388 | 91.741 | 32.008 | 56.561 | 1.00 | 39.83 |
| | 3672 | H | THR | 388 | 88.782 | 34.613 | 55.129 | 1.00 | 25.00 |
| | 3673 | HG1 | THR | 388 | 91.243 | 33.885 | 58.206 | 1.00 | 25.00 |
| | 3674 | N | PRO | 389 | 90.575 | 32.649 | 52.761 | 1.00 | 34.93 |
| | 3675 | CA | PRO | 389 | 90.184 | 31.645 | 51.769 | 1.00 | 34.82 |
| 45 | 3676 | C | PRO | 389 | 90.846 | 30.293 | 51.974 | 1.00 | 39.00 |
| | 3677 | O | PRO | 389 | 91.864 | 30.185 | 52.658 | 1.00 | 44.20 |
| | 3678 | CB | PRO | 389 | 90.654 | 32.273 | 50.460 | 1.00 | 29.22 |
| | 3679 | CG | PRO | 389 | 91.878 | 33.003 | 50.869 | 1.00 | 31.21 |
| | 3680 | CD | PRO | 389 | 91.444 | 33.671 | 52.151 | 1.00 | 33.29 |
| 50 | 3681 | N | PRO | 390 | 90.243 | 29.231 | 51.425 | 1.00 | 39.35 |
| | 3682 | CA | PRO | 390 | 90.830 | 27.896 | 51.566 | 1.00 | 38.80 |
| | 3683 | C | PRO | 390 | 92.130 | 27.894 | 50.744 | 1.00 | 42.47 |

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|----|------|-----|-----|-----|---------|--------|---------|------|-------|
| | 3684 | O | PRO | 390 | 92.264 | 28.683 | 49.801 | 1.00 | 41.59 |
| | 3685 | CB | PRO | 390 | 89.756 | 26.991 | 50.960 | 1.00 | 35.31 |
| | 3686 | CG | PRO | 390 | 89.094 | 27.876 | 49.944 | 1.00 | 39.05 |
| | 3687 | CD | PRO | 390 | 88.968 | 29.177 | 50.690 | 1.00 | 35.38 |
| 5 | 3688 | N | VAL | 391 | 93.070 | 27.015 | 51.085 | 1.00 | 42.92 |
| | 3689 | CA | VAL | 391 | 94.367 | 26.947 | 50.396 | 1.00 | 40.91 |
| | 3690 | C | VAL | 391 | 94.310 | 27.035 | 48.869 | 1.00 | 40.48 |
| | 3691 | O | VAL | 391 | 95.026 | 27.832 | 48.266 | 1.00 | 37.26 |
| | 3692 | CB | VAL | 391 | 95.163 | 25.685 | 50.800 | 1.00 | 42.01 |
| 10 | 3693 | CG1 | VAL | 391 | 96.542 | 25.698 | 50.149 | 1.00 | 37.12 |
| | 3694 | CG2 | VAL | 391 | 95.298 | 25.616 | 52.307 | 1.00 | 37.77 |
| | 3695 | H | VAL | 391 | 92.886 | 26.404 | 51.823 | 1.00 | 25.00 |
| | 3696 | N | SER | 392 | 93.455 | 26.228 | 48.251 | 1.00 | 37.92 |
| | 3697 | CA | SER | 392 | 93.316 | 26.223 | 46.799 | 1.00 | 36.67 |
| 15 | 3698 | C | SER | 392 | 93.065 | 27.627 | 46.253 | 1.00 | 37.70 |
| | 3699 | O | SER | 392 | 93.699 | 28.056 | 45.289 | 1.00 | 39.57 |
| | 3700 | CB | SER | 392 | 92.167 | 25.301 | 46.399 | 1.00 | 41.29 |
| | 3701 | OG | SER | 392 | 91.008 | 25.599 | 47.163 | 1.00 | 53.55 |
| | 3702 | H | SER | 392 | 92.894 | 25.625 | 48.776 | 1.00 | 25.00 |
| 20 | 3703 | HG | SER | 392 | 90.720 | 26.495 | 46.965 | 1.00 | 25.00 |
| | 3704 | N | GLU | 393 | 92.140 | 28.342 | 46.883 | 1.00 | 35.95 |
| | 3705 | CA | GLU | 393 | 91.806 | 29.692 | 46.455 | 1.00 | 34.88 |
| | 3706 | C | GLU | 393 | 92.951 | 30.643 | 46.783 | 1.00 | 31.14 |
| | 3707 | O | GLU | 393 | 93.293 | 31.516 | 45.984 | 1.00 | 29.96 |
| 25 | 3708 | CB | GLU | 393 | 90.518 | 30.159 | 47.130 | 1.00 | 35.59 |
| | 3709 | CG | GLU | 393 | 89.956 | 31.447 | 46.559 | 1.00 | 35.57 |
| | 3710 | CD | GLU | 393 | 88.745 | 31.951 | 47.318 | 1.00 | 39.64 |
| | 3711 | OE1 | GLU | 393 | 88.064 | 31.141 | 47.985 | 1.00 | 40.88 |
| | 3712 | OE2 | GLU | 393 | 88.475 | 33.167 | 47.2242 | 1.00 | 40.96 |
| 30 | 3713 | H | GLU | 393 | 91.694 | 27.967 | 47.669 | 1.00 | 25.00 |
| | 3714 | N | TYR | 394 | 93.539 | 30.476 | 47.962 | 1.00 | 32.04 |
| | 3715 | CA | TYR | 394 | 94.655 | 31.318 | 48.371 | 1.00 | 29.74 |
| | 3716 | C | TYR | 394 | 95.743 | 31.287 | 47.302 | 1.00 | 31.70 |
| | 3717 | O | TYR | 394 | 96.180 | 32.335 | 46.822 | 1.00 | 33.06 |
| 35 | 3718 | CB | TYR | 394 | 95.238 | 30.844 | 49.706 | 1.00 | 33.01 |
| | 3719 | CG | TYR | 394 | 96.546 | 31.520 | 50.059 | 1.00 | 42.08 |
| | 3720 | CD1 | TYR | 394 | 96.585 | 32.876 | 50.392 | 1.00 | 45.51 |
| | 3721 | CD2 | TYR | 394 | 97.752 | 30.815 | 50.021 | 1.00 | 35.80 |
| | 3722 | CE1 | TYR | 394 | 97.791 | 33.517 | 50.675 | 1.00 | 45.10 |
| 40 | 3723 | CE2 | TYR | 394 | 98.963 | 31.448 | 50.299 | 1.00 | 36.76 |
| | 3724 | CZ | TYR | 394 | 98.975 | 32.798 | 50.627 | 1.00 | 42.58 |
| | 3725 | OH | TYR | 394 | 100.164 | 33.430 | 50.915 | 1.00 | 41.43 |
| | 3726 | H | TYR | 394 | 93.225 | 29.778 | 48.567 | 1.00 | 25.00 |
| | 3727 | HH | TYR | 394 | 99.991 | 34.360 | 51.082 | 1.00 | 25.00 |
| 45 | 3728 | N | LEU | 395 | 96.145 | 30.082 | 46.909 | 1.00 | 28.83 |
| | 3729 | CA | LEU | 395 | 97.189 | 29.897 | 45.910 | 1.00 | 26.16 |
| | 3730 | C | LEU | 395 | 96.865 | 30.472 | 44.541 | 1.00 | 29.12 |
| | 3731 | O | LEU | 395 | 97.737 | 31.063 | 43.901 | 1.00 | 28.83 |
| | 3732 | CB | LEU | 395 | 97.550 | 28.415 | 45.770 | 1.00 | 28.06 |
| 50 | 3733 | CG | LEU | 395 | 98.263 | 27.754 | 46.951 | 1.00 | 27.93 |
| | 3734 | CD1 | LEU | 395 | 98.511 | 26.290 | 46.636 | 1.00 | 28.97 |
| | 3735 | CD2 | LEU | 395 | 99.575 | 28.475 | 47.245 | 1.00 | 24.02 |

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|----|------|------|-----|-----|---------|--------|--------|------|-------|
| | 3736 | H | LEU | 395 | 95.720 | 29.293 | 47.301 | 1.00 | 25.00 |
| | 3737 | N | SER | 396 | 95.620 | 30.324 | 44.093 | 1.00 | 29.97 |
| | 3738 | CA | SER | 396 | 95.239 | 30.836 | 42.780 | 1.00 | 32.88 |
| | 3739 | C | SER | 396 | 95.535 | 32.329 | 42.624 | 1.00 | 28.77 |
| 5 | 3740 | O | SER | 396 | 95.715 | 32.818 | 41.508 | 1.00 | 27.80 |
| | 3741 | CB | SER | 396 | 93.770 | 30.518 | 42.465 | 1.00 | 39.24 |
| | 3742 | OG | SER | 396 | 92.896 | 30.992 | 43.472 | 1.00 | 46.99 |
| | 3743 | H | SER | 396 | 94.943 | 29.866 | 44.642 | 1.00 | 25.00 |
| | 3744 | HG | SER | 396 | 92.971 | 31.948 | 43.546 | 1.00 | 25.00 |
| 10 | 3745 | N | ASN | 397 | 95.597 | 33.046 | 43.745 | 1.00 | 25.18 |
| | 3746 | CA | ASN | 397 | 95.907 | 34.472 | 43.723 | 1.00 | 29.15 |
| | 3747 | C | ASN | 397 | 97.333 | 34.739 | 44.226 | 1.00 | 27.87 |
| | 3748 | O | ASN | 397 | 98.106 | 35.459 | 43.588 | 1.00 | 28.50 |
| | 3749 | CB | ASN | 397 | 94.909 | 35.264 | 44.577 | 1.00 | 29.41 |
| 15 | 3750 | CG | ASN | 397 | 95.146 | 36.770 | 44.505 | 1.00 | 35.89 |
| | 3751 | OD1 | ASN | 397 | 94.831 | 37.404 | 43.502 | 1.00 | 37.46 |
| | 3752 | ND2 | ASN | 397 | 95.715 | 37.343 | 45.564 | 1.00 | 30.17 |
| | 3753 | H | ASN | 397 | 95.421 | 32.602 | 44.603 | 1.00 | 25.00 |
| | 3754 | 1HD2 | ASN | 397 | 95.872 | 38.310 | 45.510 | 1.00 | 25.00 |
| 20 | 3755 | 2HD2 | ASN | 397 | 95.953 | 36.794 | 46.336 | 1.00 | 25.00 |
| | 3756 | N | ALA | 398 | 97.682 | 34.123 | 45.351 | 1.00 | 26.89 |
| | 3757 | CA | ALA | 398 | 98.986 | 34.300 | 45.980 | 1.00 | 24.87 |
| | 3758 | C | ALA | 398 | 100.205 | 33.854 | 45.178 | 1.00 | 28.89 |
| | 3759 | O | ALA | 398 | 101.303 | 34.358 | 45.395 | 1.00 | 31.67 |
| 25 | 3760 | CB | ALA | 398 | 98.992 | 33.646 | 47.337 | 1.00 | 24.15 |
| | 3761 | H | ALA | 398 | 97.035 | 33.533 | 45.770 | 1.00 | 25.00 |
| | 3762 | N | LEU | 399 | 100.039 | 32.910 | 44.262 | 1.00 | 27.33 |
| | 3763 | CA | LEU | 399 | 101.181 | 32.464 | 43.474 | 1.00 | 29.45 |
| | 3764 | C | LEU | 399 | 101.755 | 33.589 | 42.617 | 1.00 | 32.27 |
| 30 | 3765 | O | LEU | 399 | 102.967 | 33.807 | 42.603 | 1.00 | 34.30 |
| | 3766 | CB | LEU | 399 | 100.823 | 31.254 | 42.611 | 1.00 | 25.44 |
| | 3767 | CG | LEU | 399 | 100.621 | 29.949 | 43.390 | 1.00 | 24.86 |
| | 3768 | CD1 | LEU | 399 | 100.172 | 28.853 | 42.451 | 1.00 | 20.68 |
| | 3769 | CD2 | LEU | 399 | 101.900 | 29.549 | 44.104 | 1.00 | 22.68 |
| 35 | 3770 | H | LEU | 399 | 99.159 | 32.500 | 44.121 | 1.00 | 25.00 |
| | 3771 | N | ALA | 400 | 100.887 | 34.336 | 41.943 | 1.00 | 29.07 |
| | 3772 | CA | ALA | 400 | 101.343 | 35.434 | 41.094 | 1.00 | 31.03 |
| | 3773 | C | ALA | 400 | 101.939 | 36.601 | 41.882 | 1.00 | 29.34 |
| | 3774 | O | ALA | 400 | 102.813 | 37.303 | 41.373 | 1.00 | 26.86 |
| 40 | 3775 | CB | ALA | 400 | 100.215 | 35.925 | 40.192 | 1.00 | 32.40 |
| | 3776 | H | ALA | 400 | 99.932 | 34.143 | 42.022 | 1.00 | 25.00 |
| | 3777 | N | THR | 401 | 101.500 | 36.796 | 43.125 | 1.00 | 27.66 |
| | 3778 | CA | THR | 401 | 102.024 | 37.896 | 43.929 | 1.00 | 30.92 |
| | 3779 | C | THR | 401 | 103.505 | 37.728 | 44.303 | 1.00 | 35.35 |
| 45 | 3780 | O | THR | 401 | 104.118 | 38.649 | 44.847 | 1.00 | 36.05 |
| | 3781 | CB | THR | 401 | 101.170 | 38.174 | 45.194 | 1.00 | 27.88 |
| | 3782 | OG1 | THR | 401 | 101.106 | 37.007 | 46.021 | 1.00 | 27.11 |
| | 3783 | CG2 | THR | 401 | 99.768 | 38.593 | 44.803 | 1.00 | 25.60 |
| | 3784 | H | THR | 401 | 100.837 | 36.193 | 43.521 | 1.00 | 25.00 |
| 50 | 3785 | HG1 | THR | 401 | 101.990 | 36.769 | 46.324 | 1.00 | 25.00 |
| | 3786 | N | THR | 402 | 104.076 | 36.558 | 44.016 | 1.00 | 30.98 |
| | 3787 | CA | THR | 402 | 105.492 | 36.310 | 44.295 | 1.00 | 28.76 |

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|----|------|-----|-----|------|---------|--------|--------|------|-------|
| | 3788 | C | THR | 402 | 106.317 | 37.040 | 43.240 | 1.00 | 28.41 |
| | 3789 | O | THR | 402 | 107.509 | 37.248 | 43.422 | 1.00 | 30.86 |
| | 3790 | CB | THR | 402 | 105.861 | 34.807 | 44.173 | 1.00 | 24.70 |
| | 3791 | OG1 | THR | 402 | 105.656 | 34.372 | 42.820 | 1.00 | 22.39 |
| 5 | 3792 | CG2 | THR | 402 | 105.039 | 33.954 | 45.117 | 1.00 | 21.26 |
| | 3793 | H | THR | 402 | 103.554 | 35.829 | 43.612 | 1.00 | 25.00 |
| | 3794 | HG1 | THR | 402 | 105.851 | 33.431 | 42.770 | 1.00 | 25.00 |
| | 3795 | N | THR | 403 | 105.656 | 37.373 | 42.130 | 1.00 | 28.49 |
| | 3796 | CA | THR | 403 | 106.207 | 38.045 | 40.946 | 1.00 | 25.51 |
| 10 | 3797 | C | THR | 403 | 107.032 | 37.101 | 40.077 | 1.00 | 27.25 |
| | 3798 | O | THR | 403 | 107.499 | 37.495 | 39.009 | 1.00 | 29.50 |
| | 3799 | CB | THR | 403 | 107.060 | 39.323 | 41.246 | 1.00 | 29.54 |
| | 3800 | OG1 | THR | 403 | 108.335 | 38.954 | 41.781 | 1.00 | 24.64 |
| | 3801 | CG2 | THR | 403 | 106.339 | 40.267 | 42.203 | 1.00 | 26.87 |
| 15 | 3802 | H | THR | 403 | 104.707 | 37.143 | 42.086 | 1.00 | 25.00 |
| | 3803 | HG1 | THR | 403 | 108.246 | 38.543 | 42.630 | 1.00 | 25.00 |
| | 3804 | N | TYR | 404 | 107.120 | 35.833 | 40.474 | 1.00 | 25.89 |
| | 3805 | CA | TYR | 404 | 107.914 | 34.860 | 39.728 | 1.00 | 22.27 |
| | 3806 | C | TYR | 404 | 107.544 | 34.611 | 38.272 | 1.00 | 24.30 |
| 20 | 3807 | O | TYR | 404 | 108.439 | 34.511 | 37.434 | 1.00 | 26.21 |
| | 3808 | CB | TYR | 404 | 108.062 | 33.551 | 40.509 | 1.00 | 30.29 |
| | 3809 | CG | TYR | 404 | 109.278 | 33.544 | 41.419 | 1.00 | 30.18 |
| | 3810 | CD1 | TYR | 404 | 109.800 | 34.736 | 41.922 | 1.00 | 31.88 |
| | 3811 | CD2 | TYR | 404 | 109.925 | 32.352 | 41.755 | 1.00 | 28.35 |
| 25 | 3812 | CE1 | TYR | 404 | 110.937 | 34.747 | 42.732 | 1.00 | 30.99 |
| | 3813 | CE2 | TYR | 404 | 111.065 | 32.353 | 42.569 | 1.00 | 29.01 |
| | 3814 | CZ | TYR | 404 | 111.563 | 33.558 | 43.051 | 1.00 | 29.70 |
| | 3815 | OH | TYR | 404 | 112.683 | 33.593 | 43.847 | 1.00 | 27.42 |
| | 3816 | H | TYR | 404 | 106.644 | 35.551 | 41.285 | 1.00 | 25.00 |
| 30 | 3817 | HH | TYR | 404 | 113.022 | 32.697 | 43.955 | 1.00 | 25.00 |
| | 3818 | N | TYR | 405 | 106.253 | 34.508 | 37.952 | 1.00 | 24.23 |
| | 3819 | CA | TYR | 405 | 105.844 | 34.306 | 36.553 | 1.00 | 24.60 |
| | 3820 | C | TYR | 405 | 106.361 | 35.507 | 35.766 | 1.00 | 23.35 |
| | 3821 | O | TYR | 405 | 106.912 | 35.378 | 34.672 | 1.00 | 23.93 |
| 35 | 3822 | CB | TYR | 405 | 104.317 | 34.292 | 36.406 | 1.00 | 25.23 |
| | 3823 | CG | TYR | 405 | 103.593 | 33.163 | 37.099 | 1.00 | 24.35 |
| | 3824 | CD1 | TYR | 405 | 103.561 | 31.879 | 36.548 | 1.00 | 23.45 |
| | 3825 | CD2 | TYR | 405 | 102.894 | 33.390 | 38.282 | 1.00 | 23.55 |
| | 3826 | CE1 | TYR | 4005 | 102.846 | 30.852 | 37.161 | 1.00 | 23.28 |
| 40 | 3827 | CE2 | TYR | 405 | 102.179 | 32.374 | 38.901 | 1.00 | 27.86 |
| | 3828 | CZ | TYR | 405 | 102.155 | 31.111 | 38.337 | 1.00 | 26.80 |
| | 3829 | OH | TYR | 405 | 101.428 | 30.121 | 38.956 | 1.00 | 26.06 |
| | 3830 | H | TYR | 405 | 105.577 | 34.557 | 38.658 | 1.00 | 25.00 |
| | 3831 | HH | TYR | 405 | 101.510 | 29.308 | 38.452 | 1.00 | 25.00 |
| 45 | 3832 | N | TYR | 406 | 106.160 | 36.676 | 36.363 | 1.00 | 23.37 |
| | 3833 | CA | TYR | 406 | 106.553 | 37.964 | 35.813 | 1.00 | 21.93 |
| | 3834 | C | TYR | 406 | 108.072 | 38.084 | 35.621 | 1.00 | 25.55 |
| | 3835 | O | TYR | 406 | 108.535 | 38.439 | 34.538 | 1.00 | 24.19 |
| | 3836 | CB | TYR | 406 | 106.021 | 39.047 | 36.751 | 1.00 | 22.96 |
| 50 | 3837 | CG | TYR | 406 | 106.379 | 40.468 | 36.408 | 1.00 | 21.90 |
| | 3838 | CD1 | TYR | 406 | 106.352 | 40.926 | 35.093 | 1.00 | 20.58 |
| | 3839 | CD2 | TYR | 406 | 106.703 | 41.375 | 37.416 | 1.00 | 27.70 |

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|----|------|-----|-----|-----|----------|--------|--------|------|-------|
| | 3840 | CE1 | TYR | 406 | 106.634 | 42.252 | 34.796 | 1.00 | 21.17 |
| | 3841 | CE2 | TYR | 406 | 106.985 | 42.700 | 37.128 | 1.00 | 24.51 |
| | 3842 | CZ | TYR | 406 | 106.947 | 43.131 | 35.820 | 1.00 | 23.02 |
| | 3843 | OH | TYR | 406 | 107.207 | 44.449 | 35.541 | 1.00 | 28.99 |
| 5 | 3844 | H | TYR | 406 | 105.729 | 36.670 | 37.238 | 1.00 | 25.00 |
| | 3845 | HH | TYR | 406 | 107.398 | 44.923 | 36.351 | 1.00 | 25.00 |
| | 3846 | N | LEU | 407 | 108.844 | 37.750 | 36.652 | 1.00 | 25.38 |
| | 3847 | CA | LEU | 407 | 110.303 | 37.826 | 36.574 | 1.00 | 23.31 |
| | 3848 | C | LEU | 407 | 110.873 | 36.825 | 35.575 | 1.00 | 20.18 |
| 10 | 3849 | O | LEU | 407 | 111.803 | 37.147 | 34.836 | 1.00 | 22.15 |
| | 3850 | CB | LEU | 407 | 110.940 | 37.620 | 37.952 | 1.00 | 20.82 |
| | 3851 | CG | LEU | 407 | 110.514 | 38.602 | 39.048 | 1.00 | 25.79 |
| | 3852 | CD1 | LEU | 407 | 111.362 | 38.376 | 40.287 | 1.00 | 24.12 |
| | 3853 | CD2 | LEU | 407 | 110.636 | 40.045 | 38.562 | 1.00 | 15.72 |
| 15 | 3854 | H | LEU | 407 | 108.434 | 37.445 | 37.475 | 1.00 | 25.00 |
| | 3855 | N | ALA | 408 | 110.299 | 35.625 | 35.539 | 1.00 | 14.35 |
| | 3856 | CA | ALA | 408 | 110.747 | 34.591 | 34.609 | 1.00 | 17.38 |
| | 3857 | C | ALA | 408 | 110.520 | 35.083 | 33.183 | 1.00 | 22.75 |
| | 3858 | O | ALA | 408 | 111.382 | 34.931 | 32.318 | 1.00 | 25.21 |
| 20 | 3859 | CB | ALA | 408 | 109.991 | 33.293 | 34.852 | 1.00 | 17.26 |
| | 3860 | H | ALA | 408 | 109.560 | 35.429 | 36.149 | 1.00 | 25.00 |
| | 3861 | N | THR | 409 | 109.362 | 35.695 | 32.949 | 1.00 | 23.86 |
| | 3862 | CA | THR | 409 | 109.037 | 36.228 | 31.632 | 1.00 | 22.93 |
| | 3863 | C | THR | 409 | 110.012 | 37.353 | 31.294 | 1.00 | 25.61 |
| 25 | 3864 | O | THR | 409 | 110.507 | 37.443 | 30.165 | 1.00 | 26.75 |
| | 3865 | CB | THR | 409 | 107.598 | 36.776 | 31.589 | 1.00 | 26.26 |
| | 3866 | OG1 | THR | 409 | 106.689 | 35.765 | 32.042 | 1.00 | 26.48 |
| | 3867 | CG2 | THR | 409 | 107.222 | 37.170 | 30.173 | 1.00 | 18.58 |
| | 3868 | H | THR | 409 | 108.709 | 35.780 | 33.672 | 1.00 | 25.00 |
| 30 | 3869 | HG1 | THR | 409 | 106.917 | 35.516 | 32.932 | 1.00 | 25.00 |
| | 3870 | N | THR | 410 | 110.316 | 38.185 | 32.287 | 1.00 | 26.70 |
| | 3871 | CA | THR | 410 | 111.233 | 39.299 | 32.095 | 1.00 | 26.67 |
| | 3872 | C | THR | 410 | 112.650 | 38.835 | 31.757 | 1.00 | 29.09 |
| | 3873 | O | THR | 410 | 113.298 | 39.411 | 30.877 | 1.00 | 29.16 |
| 35 | 3874 | CB | THR | 410 | 111.281 | 40.208 | 33.333 | 1.00 | 28.30 |
| | 3875 | OG1 | THR | 410 | 109.962 | 40.684 | 33.626 | 1.00 | 30.05 |
| | 3876 | CG2 | THR | 410 | 112.189 | 41.404 | 33.082 | 1.00 | 28.81 |
| | 3877 | H | THR | 410 | 109.905 | 38.064 | 33.169 | 1.00 | 25.00 |
| | 3878 | HG1 | THR | 410 | 109.991 | 41.259 | 34.393 | 1.00 | 25.00 |
| 40 | 3879 | N | SER | 411 | 113.105 | 37.760 | 32.399 | 1.00 | 24.71 |
| | 3880 | CA | SER | 411 | 114.452 | 37.254 | 32.155 | 1.00 | 24.18 |
| | 3881 | C | SER | 411 | 114.688 | 36.909 | 30.687 | 1.00 | 25.08 |
| | 3882 | O | SER | 411 | 115.822 | 36.964 | 30.204 | 1.00 | 27.75 |
| | 3883 | CB | SER | 411 | 114.753 | 36.046 | 33.043 | 1.00 | 20.40 |
| 45 | 3884 | OG | SER | 411 | 114.010 | 34.914 | 32.644 | 1.00 | 21.48 |
| | 3885 | H | SER | 411 | 112.534 | 37.287 | 33.041 | 1.00 | 25.00 |
| | 3886 | HG | SER | 411 | 114.205 | 34.667 | 31.738 | 1.00 | 25.00 |
| | 3887 | N | TYR | 412 | 113.613 | 36.573 | 29.979 | 1.00 | 23.79 |
| | 3888 | CA | TYR | 412 | 113.692 | 36.227 | 28.562 | 1.00 | 24.39 |
| 50 | 3889 | C | TYR | 412 | 113.8774 | 37.44 | 27.655 | 1.00 | 25.24 |
| | 3890 | O | TYR | 412 | 114.437 | 37.326 | 26.570 | 1.00 | 27.76 |
| | 3891 | CB | TYR | 412 | 112.419 | 35.511 | 28.116 | 1.00 | 25.37 |

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|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 3892 | CG | TYR | 412 | 112.273 | 34.072 | 28.539 | 1.00 | 29.38 |
| | 3893 | CD1 | TYR | 412 | 113.043 | 33.531 | 29.569 | 1.00 | 29.32 |
| | 3894 | CD2 | TYR | 412 | 111.338 | 33.248 | 27.910 | 1.00 | 24.28 |
| | 3895 | CE1 | TYR | 412 | 112.878 | 32.199 | 29.964 | 1.00 | 26.36 |
| 5 | 3896 | CE2 | TYR | 412 | 111.169 | 31.927 | 28.291 | 1.00 | 25.08 |
| | 3897 | CZ | TYR | 412 | 111.937 | 31.408 | 29.318 | 1.00 | 29.45 |
| | 3898 | OH | TYR | 412 | 111.750 | 30.099 | 29.693 | 1.00 | 27.61 |
| | 3899 | H | TYR | 412 | 112.738 | 36.552 | 30.423 | 1.00 | 25.00 |
| | 3900 | HH | TYR | 412 | 112.347 | 29.879 | 30.418 | 1.00 | 25.00 |
| 10 | 3901 | N | LEU | 413 | 113.396 | 38.604 | 28.100 | 1.00 | 25.11 |
| | 3902 | CA | LEU | 413 | 113.467 | 39.832 | 27.304 | 1.00 | 27.32 |
| | 3903 | C | LEU | 413 | 114.835 | 40.149 | 26.726 | 1.00 | 30.49 |
| | 3904 | O | LEU | 413 | 114.957 | 40.434 | 25.533 | 1.00 | 30.50 |
| | 3905 | CB | LEU | 413 | 112.959 | 41.039 | 28.103 | 1.00 | 23.58 |
| 15 | 3906 | CG | LEU | 413 | 111.476 | 41.081 | 28.478 | 1.00 | 31.45 |
| | 3907 | CD1 | LEU | 413 | 111.179 | 42.362 | 29.242 | 1.00 | 31.49 |
| | 3908 | CD2 | LEU | 413 | 110.613 | 40.996 | 27.231 | 1.00 | 30.34 |
| | 3909 | H | LEU | 413 | 112.980 | 38.636 | 28.989 | 1.00 | 25.00 |
| | 3910 | N | GLY | 414 | 115.859 | 40.098 | 27.573 | 1.00 | 28.96 |
| 20 | 3911 | CA | GLY | 414 | 117.203 | 40.404 | 27.129 | 1.00 | 27.47 |
| | 3912 | C | GLY | 414 | 117.990 | 39.233 | 26.586 | 1.00 | 28.88 |
| | 3913 | O | GLY | 414 | 119.186 | 39.362 | 26.340 | 1.00 | 34.59 |
| | 3914 | H | GLY | 414 | 115.698 | 39.833 | 28.496 | 1.00 | 25.00 |
| | 3915 | N | MET | 415 | 117.353 | 38.079 | 26.436 | 1.00 | 29.79 |
| 25 | 3916 | CA | MET | 415 | 118.043 | 36.909 | 25.906 | 1.00 | 29.75 |
| | 3917 | C | MET | 415 | 117.861 | 36.868 | 24.393 | 1.00 | 35.70 |
| | 3918 | O | MET | 415 | 116.795 | 36.522 | 23.893 | 1.00 | 39.21 |
| | 3919 | CB | MET | 415 | 117.515 | 35.630 | 26.554 | 1.00 | 22.67 |
| | 3920 | CG | MET | 415 | 117.728 | 35.581 | 28.050 | 1.00 | 23.60 |
| 30 | 3921 | SD | MET | 415 | 117.062 | 34.095 | 28.794 | 1.00 | 32.91 |
| | 3922 | CE | MET | 415 | 118.255 | 32.896 | 28.242 | 1.00 | 24.83 |
| | 3923 | H | MET | 415 | 116.398 | 38.012 | 26.652 | 1.00 | 25.00 |
| | 3924 | N | LYS | 416 | 118.933 | 37.181 | 23.677 | 1.00 | 40.25 |
| | 3925 | CA | LYS | 416 | 118.942 | 37.233 | 22.218 | 1.00 | 43.20 |
| 35 | 3926 | C | LYS | 416 | 118.370 | 36.031 | 21.466 | 1.00 | 42.08 |
| | 3927 | O | LYS | 416 | 118.037 | 36.143 | 20.289 | 1.00 | 44.24 |
| | 3928 | CB | LYS | 416 | 120.362 | 37.539 | 21.735 | 1.00 | 48.69 |
| | 3929 | CG | LYS | 416 | 120.916 | 38.828 | 22.333 | 1.00 | 60.37 |
| | 3930 | CD | LYS | 416 | 122.427 | 38.949 | 22.191 | 1.00 | 70.42 |
| 40 | 3931 | CE | LYS | 416 | 122.936 | 40.173 | 22.949 | 1.00 | 72.06 |
| | 3932 | NZ | LYS | 416 | 124.412 | 40.319 | 22.863 | 1.00 | 78.00 |
| | 3933 | H | LYS | 416 | 119.749 | 37.416 | 24.164 | 1.00 | 25.00 |
| | 3934 | 1HZ | LYS | 416 | 124.870 | 39.475 | 23.262 | 1.00 | 25.00 |
| | 3935 | 2HZ | LYS | 416 | 124.687 | 40.423 | 21.865 | 1.00 | 25.00 |
| 45 | 3936 | 3HZ | LYS | 416 | 124.709 | 41.163 | 23.393 | 1.00 | 25.00 |
| | 3937 | N | SER | 417 | 118.239 | 34.893 | 22.138 | 1.00 | 39.46 |
| | 3938 | CA | SER | 417 | 117.706 | 33.698 | 21.491 | 1.00 | 36.96 |
| | 3939 | C | SER | 417 | 116.247 | 33.395 | 21.833 | 1.00 | 34.08 |
| | 3940 | O | SER | 417 | 115.637 | 32.518 | 21.226 | 1.00 | 35.80 |
| 50 | 3941 | CB | SER | 417 | 118.580 | 32.488 | 21.823 | 1.00 | 39.51 |
| | 3942 | OG | SER | 417 | 119.907 | 32.675 | 21.358 | 1.00 | 45.86 |
| | 3943 | H | SER | 417 | 118.485 | 34.856 | 23.077 | 1.00 | 25.00 |

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|----|------|------|-----|-----|---------|--------|---------|------|-------|
| | 3944 | HG | SER | 417 | 120.288 | 33.461 | 21.743 | 1.00 | 25.00 |
| | 3945 | N | ALA | 418 | 115.688 | 34.106 | 22.806 | 1.00 | 30.28 |
| | 3946 | CA | ALA | 418 | 114.303 | 33.879 | 23.208 | 1.00 | 38.39 |
| | 3947 | C | ALA | 418 | 113.331 | 34.250 | 22.087 | 1.00 | 40.58 |
| 5 | 3948 | O | ALA | 418 | 113.145 | 35.427 | 21.779 | 1.00 | 42.57 |
| | 3949 | CB | ALA | 418 | 113.981 | 34.659 | 24.484 | 1.00 | 32.32 |
| | 3950 | H | ALA | 418 | 116.190 | 34.823 | 23.238 | 1.00 | 25.00 |
| | 3951 | N | THR | 419 | 112.750 | 33.232 | 21.457 | 1.00 | 41.43 |
| | 3952 | CA | THR | 419 | 111.799 | 33.420 | 220.362 | 1.00 | 41.21 |
| 10 | 3953 | C | THR | 419 | 110.357 | 33.504 | 20.865 | 1.00 | 40.11 |
| | 3954 | O | THR | 419 | 110.077 | 33.235 | 22.036 | 1.00 | 39.88 |
| | 3955 | CB | THR | 419 | 111.892 | 32.264 | 19.338 | 1.00 | 39.89 |
| | 3956 | OG1 | THR | 419 | 111.666 | 31.016 | 20.005 | 1.00 | 50.18 |
| | 3957 | CG2 | THR | 419 | 113.261 | 32.238 | 18.672 | 1.00 | 37.82 |
| 15 | 3958 | H | THR | 419 | 112.987 | 32.335 | 21.728 | 1.00 | 25.00 |
| | 3959 | HG1 | THR | 419 | 112.370 | 30.881 | 20.644 | 1.00 | 25.00 |
| | 3960 | N | GLU | 420 | 109.443 | 33.848 | 19.963 | 1.00 | 39.64 |
| | 3961 | CA | GLU | 420 | 108.027 | 33.958 | 20.292 | 1.00 | 39.75 |
| | 3962 | C | GLU | 420 | 107.496 | 32.650 | 20.871 | 1.00 | 35.49 |
| 20 | 3963 | O | GLU | 420 | 106.718 | 32.652 | 21.828 | 1.00 | 35.76 |
| | 3964 | CB | GLU | 420 | 107.222 | 34.321 | 19.041 | 1.00 | 46.65 |
| | 3965 | CG | GLU | 420 | 106.741 | 35.765 | 18.980 | 1.00 | 56.30 |
| | 3966 | CD | GLU | 420 | 105.668 | 36.081 | 20.015 | 1.00 | 65.12 |
| | 3967 | OE1 | GLU | 420 | 104.685 | 35.311 | 20.130 | 1.00 | 62.03 |
| 25 | 3968 | OE2 | GLU | 420 | 105.804 | 37.112 | 20.707 | 1.00 | 72.02 |
| | 3969 | H | GLU | 420 | 109.732 | 34.021 | 19.047 | 1.00 | 25.00 |
| | 3970 | N | GLN | 421 | 107.938 | 31.537 | 20.291 | 1.00 | 32.71 |
| | 3971 | CA | GLN | 421 | 107.520 | 30.206 | 20.722 | 1.00 | 36.14 |
| | 3972 | C | GLN | 421 | 107.883 | 29.959 | 22.184 | 1.00 | 36.63 |
| 30 | 3973 | O | GLN | 421 | 107.105 | 29.365 | 22.936 | 1.00 | 37.57 |
| | 3974 | CB | GLN | 421 | 108.155 | 29.133 | 19.830 | 1.00 | 40.03 |
| | 3975 | CG | GLN | 421 | 107.622 | 29.086 | 18.398 | 1.00 | 53.07 |
| | 3976 | CD | GLN | 421 | 107.819 | 30.390 | 17.636 | 1.00 | 62.17 |
| | 3977 | OE1 | GLN | 421 | 108.877 | 31.017 | 17.711 | 1.00 | 65.66 |
| 35 | 3978 | NE2 | GLN | 421 | 106.788 | 30.815 | 16.917 | 1.00 | 68.97 |
| | 3979 | H | GLN | 421 | 108.580 | 31.620 | 19.555 | 1.00 | 25.00 |
| | 3980 | 1HE2 | GLN | 421 | 106.906 | 31.650 | 16.419 | 1.00 | 25.00 |
| | 3981 | 2HE2 | GLN | 421 | 105.963 | 30.289 | 16.903 | 1.00 | 25.00 |
| | 3982 | N | ASP | 422 | 109.052 | 30.448 | 22.589 | 1.00 | 34.98 |
| 40 | 3983 | CA | ASP | 422 | 109.521 | 30.292 | 23.960 | 1.00 | 32.53 |
| | 3984 | C | ASP | 422 | 108.607 | 31.039 | 24.924 | 1.00 | 30.54 |
| | 3985 | O | ASP | 422 | 108.272 | 30.525 | 25.992 | 1.00 | 33.81 |
| | 3986 | CB | ASP | 422 | 110.972 | 30.767 | 24.085 | 1.00 | 28.20 |
| | 3987 | CG | ASP | 422 | 111.929 | 29.945 | 23.233 | 1.00 | 28.18 |
| 45 | 3988 | OD1 | ASP | 422 | 111.755 | 28.710 | 23.148 | 1.00 | 33.24 |
| | 3989 | OD2 | ASP | 422 | 112.855 | 30.529 | 22.638 | 1.00 | 33.81 |
| | 3990 | H | ASP | 422 | 109.610 | 30.933 | 21.946 | 1.00 | 25.00 |
| | 3991 | N | PHE | 423 | 108.166 | 32.229 | 24.523 | 1.00 | 29.33 |
| | 3992 | CA | PHE | 423 | 107.261 | 33.022 | 25.348 | 1.00 | 28.15 |
| 50 | 3993 | C | PHE | 423 | 105.877 | 32.373 | 25.407 | 1.00 | 29.51 |
| | 3994 | O | PHE | 423 | 105.205 | 32.424 | 26.441 | 1.00 | 30.32 |
| | 3995 | CB | PHE | 423 | 107.143 | 34.448 | 24.808 | 1.00 | 31.32 |

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|----|-------|-----|-----|-----|---------|--------|--------|------|-------|
| | 3996 | CG | PHE | 423 | 108.275 | 35.353 | 25.214 | 1.00 | 27.99 |
| | 3997 | CD1 | PHE | 423 | 108.227 | 36.045 | 26.421 | 1.00 | 26.74 |
| | 3998 | CD2 | PHE | 423 | 109.375 | 35.529 | 24.387 | 1.00 | 26.53 |
| | 3999 | CE1 | PHE | 423 | 109.255 | 36.900 | 26.794 | 1.00 | 21.72 |
| 5 | 4000 | CE2 | PHE | 423 | 110.412 | 36.385 | 24.753 | 1.00 | 23.04 |
| | 4001 | CZ | PHE | 423 | 110.350 | 37.070 | 25.958 | 1.00 | 23.46 |
| | 4002 | H | PHE | 423 | 108.456 | 32.575 | 23.652 | 1.00 | 25.00 |
| | 40003 | N | GLU | 424 | 105.450 | 31.771 | 24.297 | 1.00 | 30.80 |
| | 4004 | CA | GLU | 424 | 104.146 | 31.107 | 24.233 | 1.00 | 36.62 |
| 10 | 4005 | C | GLU | 424 | 104.128 | 29.911 | 25.172 | 1.00 | 34.48 |
| | 4006 | O | GLU | 424 | 103.131 | 29.651 | 25.843 | 1.00 | 34.44 |
| | 4007 | CB | GLU | 424 | 103.823 | 30.661 | 22.805 | 1.00 | 42.57 |
| | 4008 | CG | GLU | 424 | 103.590 | 31.813 | 21.839 | 1.00 | 63.38 |
| | 4009 | CD | GLU | 424 | 103.322 | 31.357 | 20.414 | 1.00 | 70.12 |
| 15 | 4010 | OE1 | GLU | 424 | 103.895 | 30.329 | 19.988 | 1.00 | 72.19 |
| | 4011 | OE2 | GLU | 424 | 102.543 | 32.039 | 19.715 | 1.00 | 79.30 |
| | 4012 | H | GLU | 424 | 106.023 | 31.773 | 23.503 | 1.00 | 25.00 |
| | 4013 | N | TRP | 425 | 105.242 | 29.187 | 25.221 | 1.00 | 32.02 |
| | 4014 | CA | TRP | 425 | 105.367 | 28.038 | 26.107 | 1.00 | 28.78 |
| 20 | 4015 | C | TRP | 425 | 105.262 | 28.531 | 27.553 | 1.00 | 33.19 |
| | 4016 | O | TRP | 425 | 104.518 | 27.974 | 28.365 | 1.00 | 30.47 |
| | 4017 | CB | TRP | 425 | 106.719 | 27.352 | 25.881 | 1.00 | 29.01 |
| | 4018 | CG | TRP | 425 | 107.077 | 26.340 | 26.927 | 1.00 | 29.69 |
| | 4019 | CD1 | TRP | 425 | 106.621 | 25.058 | 27.019 | 1.00 | 28.88 |
| 25 | 4020 | CD2 | TRP | 425 | 107.970 | 26.530 | 28.034 | 1.00 | 29.87 |
| | 4021 | NE1 | TRP | 425 | 107.171 | 24.437 | 28.116 | 1.00 | 29.58 |
| | 4022 | CE2 | TRP | 425 | 108.003 | 25.316 | 28.757 | 1.00 | 32.75 |
| | 4023 | CE3 | TRP | 425 | 108.742 | 27.609 | 28.488 | 1.00 | 30.70 |
| | 4024 | CZ2 | TRP | 425 | 108.781 | 25.149 | 29.912 | 1.00 | 27.26 |
| 30 | 4025 | CZ3 | TRP | 425 | 109.514 | 27.444 | 29.638 | 1.00 | 26.04 |
| | 4026 | CH2 | TRP | 425 | 109.525 | 26.222 | 30.335 | 1.00 | 27.12 |
| | 4027 | H | TRP | 425 | 105.993 | 29.429 | 24.639 | 1.00 | 25.00 |
| | 4028 | HE1 | TRP | 425 | 106.983 | 23.517 | 28.395 | 1.00 | 25.00 |
| | 4029 | N | LEU | 426 | 105.974 | 29.615 | 27.848 | 1.00 | 31.46 |
| 35 | 4030 | CA | LEU | 426 | 105.994 | 30.186 | 29.188 | 1.00 | 28.35 |
| | 4031 | C | LEU | 426 | 104.627 | 30.692 | 29.650 | 1.00 | 31.98 |
| | 4032 | O | LEU | 426 | 104.293 | 30.585 | 30.832 | 1.00 | 29.19 |
| | 4033 | CB | LEU | 426 | 107.039 | 31.302 | 29.268 | 1.00 | 21.80 |
| | 4034 | CG | LEU | 426 | 107.525 | 31.703 | 30.664 | 1.00 | 25.44 |
| 40 | 4035 | CD1 | LEU | 426 | 108.240 | 30.535 | 31.331 | 1.00 | 20.60 |
| | 4036 | CD2 | LEU | 426 | 108.454 | 32.900 | 30.560 | 1.00 | 23.92 |
| | 4037 | H | LEU | 426 | 106.512 | 30.035 | 27.141 | 1.00 | 25.00 |
| | 4038 | N | SER | 427 | 103.824 | 31.208 | 28.720 | 1.00 | 33.95 |
| | 4039 | CA | SER | 427 | 102.497 | 31.722 | 29.066 | 1.00 | 33.39 |
| 45 | 4040 | C | SER | 427 | 101.502 | 30.647 | 29.502 | 1.00 | 30.91 |
| | 4041 | O | SER | 427 | 100.515 | 30.951 | 30.170 | 1.00 | 31.38 |
| | 4042 | CB | SER | 427 | 101.917 | 32.568 | 27.925 | 1.00 | 37.83 |
| | 4043 | OG | SER | 427 | 101.970 | 31.892 | 26.683 | 1.00 | 46.06 |
| | 4044 | H | SER | 427 | 104.124 | 31.247 | 27.790 | 1.00 | 25.00 |
| 50 | 4045 | HG | SER | 427 | 102.886 | 31.692 | 26.470 | 1.00 | 25.00 |
| | 4046 | N | LYS | 428 | 101.780 | 29.392 | 29.151 | 1.00 | 30.99 |
| | 4047 | CA | LYS | 428 | 100.914 | 28.271 | 29.518 | 1.00 | 30.38 |

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|----|------|------|-----|-----|---------|--------|--------|------|-------|
| | 4048 | C | LYS | 428 | 101.124 | 27.817 | 30.964 | 1.00 | 33.22 |
| | 4049 | O | LYS | 428 | 100.505 | 26.845 | 31.410 | 1.00 | 34.36 |
| | 4050 | CB | LYS | 428 | 101.166 | 27.070 | 28.601 | 1.00 | 33.08 |
| | 4051 | CG | LYS | 428 | 100.690 | 27.213 | 27.166 | 1.00 | 40.80 |
| 5 | 4052 | CD | LYS | 428 | 100.885 | 25.888 | 26.433 | 1.00 | 48.04 |
| | 4053 | CE | LYS | 428 | 100.314 | 25.910 | 25.002 | 1.00 | 54.20 |
| | 4054 | NZ | LYS | 428 | 100.438 | 24.571 | 24.377 | 1.00 | 59.29 |
| | 4055 | H | LYS | 428 | 102.587 | 29.209 | 28.628 | 1.00 | 25.00 |
| | 4056 | 1HZ | LYS | 428 | 99.919 | 23.866 | 24.937 | 1.00 | 25.00 |
| 10 | 4057 | 2HZ | LYS | 428 | 100.037 | 24.613 | 23.418 | 1.00 | 25.00 |
| | 4058 | 3HZ | LYS | 428 | 101.440 | 24.300 | 24.323 | 1.00 | 25.00 |
| | 4059 | N | ASN | 429 | 101.992 | 28.518 | 31.693 | 1.00 | 36.19 |
| | 4060 | CA | ASN | 429 | 102.313 | 28.172 | 33.081 | 1.00 | 31.97 |
| | 4061 | C | ASN | 429 | 102.855 | 26.740 | 33.172 | 1.00 | 29.89 |
| 15 | 4062 | O | ASN | 429 | 102.272 | 25.882 | 33.839 | 1.00 | 25.78 |
| | 4063 | CB | ASN | 429 | 101.092 | 28.334 | 33.995 | 1.00 | 32.22 |
| | 4064 | CG | ASN | 429 | 100.814 | 29.782 | 34.358 | 1.00 | 36.78 |
| | 4065 | OD1 | ASN | 429 | 101.488 | 30.699 | 33.894 | 1.00 | 40.44 |
| | 4066 | ND2 | ASN | 429 | 99.826 | 29.991 | 35.215 | 1.00 | 41.36 |
| 20 | 4067 | H | ASN | 429 | 102.436 | 29.294 | 31.299 | 1.00 | 25.00 |
| | 4068 | 1HD2 | ASN | 429 | 99.643 | 30.918 | 35.449 | 1.00 | 25.00 |
| | 4069 | 2HD2 | ASN | 429 | 99.331 | 29.226 | 35.566 | 1.00 | 25.00 |
| | 4070 | N | PRO | 430 | 103.997 | 26.472 | 32.508 | 1.00 | 29.30 |
| | 4071 | CA | PRO | 430 | 104.649 | 25.157 | 32.492 | 1.00 | 25.30 |
| 25 | 4072 | C | PRO | 430 | 104.897 | 24.669 | 33.913 | 1.00 | 27.01 |
| | 4073 | O | PRO | 430 | 105.218 | 25.463 | 34.801 | 1.00 | 27.38 |
| | 4074 | CB | PRO | 430 | 105.975 | 25.447 | 31.799 | 1.00 | 24.23 |
| | 4075 | CG | PRO | 430 | 105.664 | 26.610 | 30.932 | 1.00 | 30.06 |
| | 4076 | CD | PRO | 430 | 104.835 | 27.468 | 31.820 | 1.00 | 30.25 |
| 30 | 4077 | N | LYS | 431 | 104.824 | 23.358 | 34.108 | 1.00 | 25.65 |
| | 4078 | CA | LYS | 431 | 105.020 | 22.774 | 35.426 | 1.00 | 25.93 |
| | 4079 | C | LYS | 431 | 106.308 | 23.248 | 36.107 | 1.00 | 24.81 |
| | 4080 | O | LYS | 431 | 106.297 | 23.570 | 37.292 | 1.00 | 24.36 |
| | 4081 | CB | LYS | 431 | 105.000 | 21.252 | 35.325 | 1.00 | 26.70 |
| 35 | 4082 | CG | LYS | 431 | 104.584 | 20.547 | 36.604 | 1.00 | 40.34 |
| | 4083 | CD | LYS | 431 | 104.361 | 19.068 | 36.330 | 1.00 | 52.65 |
| | 4084 | CE | LYS | 431 | 103.775 | 18.345 | 37.531 | 1.00 | 60.92 |
| | 4085 | NZ | LYS | 431 | 103.587 | 16.892 | 37.247 | 1.00 | 58.59 |
| | 4086 | H | LYS | 431 | 104.610 | 22.777 | 33.352 | 1.00 | 25.00 |
| 40 | 4087 | 1HZ | LYS | 431 | 102.939 | 16.775 | 36.442 | 1.00 | 25.00 |
| | 4088 | 2HZ | LYS | 431 | 104.506 | 16.462 | 37.018 | 1.00 | 25.00 |
| | 4089 | 3HZ | LYS | 431 | 103.189 | 16.424 | 38.086 | 1.00 | 25.00 |
| | 4090 | N | ILE | 432 | 107.401 | 23.338 | 35.353 | 1.00 | 25.03 |
| | 4091 | CA | ILE | 432 | 108.667 | 23.774 | 35.934 | 1.00 | 21.64 |
| 45 | 4092 | C | ILE | 432 | 108.561 | 25.188 | 36.505 | 1.00 | 24.42 |
| | 4093 | O | ILE | 432 | 109.058 | 25.459 | 37.602 | 1.00 | 25.07 |
| | 4094 | CB | ILE | 432 | 109.847 | 23.646 | 34.928 | 1.00 | 22.09 |
| | 4095 | CG1 | ILE | 432 | 111.179 | 23.898 | 35.647 | 1.00 | 20.75 |
| | 4096 | CG2 | ILE | 432 | 109.662 | 24.587 | 33.739 | 1.00 | 20.53 |
| 50 | 4097 | CD1 | ILE | 432 | 112.403 | 23.511 | 34.838 | 1.00 | 17.10 |
| | 4098 | H | ILE | 432 | 107.354 | 23.103 | 34.410 | 1.00 | 25.00 |
| | 4099 | N | LEU | 433 | 107.868 | 26.070 | 35.788 | 1.00 | 25.32 |

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|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 4100 | CA | LEU | 433 | 107.674 | 27.448 | 36.240 | 1.00 | 23.97 |
| | 4101 | C | LEU | 433 | 106.758 | 27.446 | 37.464 | 1.00 | 27.11 |
| | 4102 | O | LEU | 433 | 107.051 | 28.078 | 38.483 | 1.00 | 28.11 |
| | 4103 | CB | LEU | 433 | 107.057 | 28.298 | 35.126 | 1.00 | 24.53 |
| 5 | 4104 | CG | LEU | 433 | 106.721 | 29.754 | 35.473 | 1.00 | 28.30 |
| | 4105 | CD1 | LEU | 433 | 107.968 | 30.488 | 35.945 | 1.00 | 23.75 |
| | 4106 | CD2 | LEU | 433 | 106.108 | 30.456 | 34.265 | 1.00 | 27.09 |
| | 4107 | H | LEU | 433 | 107.456 | 25.788 | 34.948 | 1.00 | 25.00 |
| | 4108 | N | GLU | 434 | 105.667 | 26.698 | 37.360 | 1.00 | 26.39 |
| 10 | 4109 | CA | GLU | 434 | 104.690 | 26.566 | 38.429 | 1.00 | 28.21 |
| | 4110 | C | GLU | 434 | 105.393 | 26.139 | 39.723 | 1.00 | 25.73 |
| | 4111 | O | GLU | 434 | 105.159 | 26.711 | 40.790 | 1.00 | 25.92 |
| | 4112 | CB | GLU | 434 | 103.656 | 25.510 | 38.027 | 1.00 | 40.62 |
| | 4113 | CG | GLU | 434 | 102.371 | 25.510 | 38.835 | 1.00 | 59.16 |
| 15 | 4114 | CD | GLU | 434 | 101.447 | 26.650 | 38.457 | 1.00 | 69.11 |
| | 4115 | OE1 | GLU | 434 | 101.135 | 26.803 | 37.255 | 1.00 | 76.28 |
| | 4116 | OE2 | GLU | 434 | 101.026 | 27.391 | 39.366 | 1.00 | 78.90 |
| | 4117 | H | GLU | 434 | 105.516 | 26.206 | 36.531 | 1.00 | 25.00 |
| | 4118 | N | ALA | 435 | 106.272 | 25.147 | 39.614 | 1.00 | 23.71 |
| 20 | 4119 | CA | ALA | 435 | 107.015 | 24.632 | 40.764 | 1.00 | 21.25 |
| | 4120 | C | ALA | 435 | 107.915 | 25.704 | 41.377 | 1.00 | 21.57 |
| | 4121 | O | ALA | 435 | 107.973 | 25.864 | 42.599 | 1.00 | 21.94 |
| | 4122 | CB | ALA | 435 | 107.838 | 23.424 | 40.353 | 1.00 | 17.11 |
| | 4123 | H | ALA | 435 | 106.427 | 24.748 | 38.737 | 1.00 | 25.00 |
| 25 | 4124 | N | SER | 436 | 108.603 | 26.448 | 40.519 | 1.00 | 20.07 |
| | 4125 | CA | SER | 436 | 109.486 | 27.510 | 40.969 | 1.00 | 21.72 |
| | 4126 | C | SER | 436 | 108.676 | 28.531 | 41.759 | 1.00 | 23.51 |
| | 4127 | O | SER | 436 | 109.095 | 28.979 | 42.832 | 1.00 | 25.11 |
| | 4128 | CB | SER | 436 | 110.147 | 28.179 | 39.765 | 1.00 | 21.38 |
| 30 | 4129 | OG | SER | 436 | 111.040 | 29.196 | 40.173 | 1.00 | 36.67 |
| | 4130 | H | SER | 436 | 108.521 | 26.272 | 39.556 | 1.00 | 25.00 |
| | 4131 | HG | SER | 436 | 110.568 | 29.867 | 40.669 | 1.00 | 25.00 |
| | 4132 | N | VAL | 437 | 107.501 | 28.876 | 41.235 | 1.00 | 23.94 |
| | 4133 | CA | VAL | 437 | 106.622 | 29.846 | 41.880 | 1.00 | 18.07 |
| 35 | 4134 | C | VAL | 437 | 106.134 | 29.330 | 43.226 | 1.00 | 19.00 |
| | 4135 | O | VAL | 437 | 106.179 | 30.048 | 44.227 | 1.00 | 24.40 |
| | 4136 | CB | VAL | 437 | 105.410 | 30.192 | 40.990 | 1.00 | 22.63 |
| | 4137 | CG1 | VAL | 437 | 104.498 | 31.163 | 41.709 | 1.00 | 24.13 |
| | 4138 | CG2 | VAL | 437 | 105.879 | 30.794 | 39.677 | 1.00 | 13.85 |
| 40 | 4139 | H | VAL | 437 | 107.218 | 28.463 | 40.391 | 1.00 | 25.00 |
| | 4140 | N | ILE | 438 | 105.693 | 28.076 | 43.249 | 1.00 | 22.97 |
| | 4141 | CA | ILE | 438 | 105.204 | 27.443 | 44.472 | 1.00 | 25.17 |
| | 4142 | C | ILE | 438 | 106.279 | 27.478 | 45.566 | 1.00 | 27.56 |
| | 4143 | O | ILE | 438 | 105.996 | 27.831 | 46.718 | 1.00 | 25.37 |
| 45 | 4144 | CB | ILE | 438 | 104.776 | 25.975 | 44.200 | 1.00 | 28.36 |
| | 4145 | CG1 | ILE | 438 | 103.565 | 25.952 | 43.262 | 1.00 | 33.63 |
| | 4146 | CG2 | ILE | 438 | 104.457 | 25.255 | 45.505 | 1.00 | 31.72 |
| | 4147 | CD1 | ILE | 438 | 103.130 | 24.569 | 42.836 | 1.00 | 33.54 |
| | 4148 | H | ILE | 438 | 105.697 | 27.559 | 42.417 | 1.00 | 25.00 |
| 50 | 4149 | N | ILE | 439 | 107.512 | 27.134 | 45.196 | 1.00 | 27.24 |
| | 4150 | CA | ILE | 439 | 108.635 | 27.130 | 46.135 | 1.00 | 24.88 |
| | 4151 | C | ILE | 439 | 108.769 | 28.502 | 46.787 | 1.00 | 20.20 |

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|----|------|------|-----|------|---------|---------|--------|------|-------|
| | 4152 | O | ILE | 439 | 108.842 | 28.610 | 48.007 | 1.00 | 20.39 |
| | 4153 | CB | ILE | 439 | 109.961 | 26.739 | 45.429 | 1.00 | 23.09 |
| | 4154 | CG1 | ILE | 439 | 109.915 | 25.264 | 45.023 | 1.00 | 21.73 |
| | 4155 | CG2 | ILE | 439 | 111.154 | 26.989 | 46.345 | 1.00 | 17.14 |
| 5 | 4156 | CD1 | ILE | 439 | 110.984 | 24.859 | 44.043 | 1.00 | 22.40 |
| | 4157 | H | ILE | 439 | 107.670 | 26.870 | 44.265 | 1.00 | 25.00 |
| | 4158 | N | CYS | 440 | 108.763 | 29.552 | 45.974 | 1.00 | 21.23 |
| | 4159 | CA | CYS | 440 | 108.873 | 30.901 | 46.508 | 1.00 | 23.58 |
| | 4160 | C | CYS | 440 | 107.718 | 31.209 | 47.458 | 1.00 | 27.42 |
| 10 | 4161 | O | CYS | 440 | 107.933 | 31.707 | 48.563 | 1.00 | 29.41 |
| | 4162 | CB | CYS | 440 | 108.897 | 31.928 | 45.376 | 1.00 | 26.26 |
| | 4163 | SG | CYS | 440 | 109.015 | 33.625 | 45.934 | 1.00 | 17.39 |
| | 4164 | H | CYS | 440 | 108.685 | 29.406 | 45.006 | 1.00 | 25.00 |
| | 4165 | N | ARG | 441 | 106.502 | 30.869 | 47.038 | 1.00 | 30.12 |
| 15 | 4166 | CA | ARG | 441 | 105.295 | 31.118 | 47.825 | 1.00 | 28.33 |
| | 4167 | C | ARG | 4441 | 105.280 | 30.448 | 49.197 | 1.00 | 28.78 |
| | 4168 | O | ARG | 441 | 105.225 | 31.125 | 50.223 | 1.00 | 28.38 |
| | 4169 | CB | ARG | 441 | 104.056 | 30.693 | 47.031 | 1.00 | 26.28 |
| | 4170 | CG | ARG | 441 | 102.722 | 30.927 | 47.734 | 1.00 | 26.09 |
| 20 | 4171 | CD | ARG | 441 | 102.312 | 32.391 | 47.725 | 1.00 | 32.68 |
| | 4172 | NE | ARG | 441 | 103.001 | 33.195 | 48.731 | 1.00 | 35.67 |
| | 4173 | CZ | ARG | 441 | 103.243 | 34.499 | 48.611 | 1.00 | 31.42 |
| | 4174 | NH1 | ARG | 441 | 102.861 | 35.159 | 47.526 | 1.00 | 25.83 |
| | 4175 | NH2 | ARG | 441 | 103.851 | 35.153 | 49.591 | 1.00 | 32.87 |
| 25 | 4176 | H | ARG | 441 | 106.413 | 30.429 | 46.165 | 1.00 | 25.00 |
| | 4177 | HE | ARG | 441 | 103.307 | 32.748 | 49.547 | 1.00 | 25.00 |
| | 4178 | 1HH1 | ARG | 441 | 102.391 | 34.678 | 46.792 | 1.00 | 25.00 |
| | 4179 | 2HH1 | ARG | 441 | 103.043 | 36.138 | 47.443 | 1.00 | 25.00 |
| | 4180 | 1HH2 | ARG | 441 | 104.133 | 34.668 | 50.417 | 1.00 | 25.00 |
| 30 | 4181 | 2HH2 | ARG | 441 | 104.032 | 36.133 | 49.498 | 1.00 | 25.00 |
| | 4182 | N | VAL | 442 | 105.329 | 29.120 | 49.220 | 1.00 | 28.03 |
| | 4183 | CA | VAL | 442 | 105.289 | 28.392 | 50.484 | 1.00 | 29.35 |
| | 4184 | C | VAL | 442 | 106.443 | 28.708 | 51.430 | 1.00 | 29.48 |
| | 4185 | O | VAL | 442 | 106.248 | 28.754 | 52.644 | 1.00 | 30.67 |
| 35 | 4186 | CB | VAL | 442 | 105.171 | 26.864 | 50.272 | 1.00 | 28.34 |
| | 4187 | CG1 | VAL | 442 | 103.906 | 26.546 | 49.489 | 1.00 | 20.42 |
| | 4188 | CG2 | VAL | 442 | 106.394 | 26.322 | 49.562 | 1.00 | 28.17 |
| | 4189 | H | VAL | 442 | 105.405 | 28.625 | 48.376 | 1.00 | 25.00 |
| | 4190 | N | ILE | 443 | 107.635 | 28.941 | 50.885 | 1.00 | 32.67 |
| 40 | 4191 | CA | ILE | 443 | 108.788 | 29.266 | 51.722 | 1.00 | 32.60 |
| | 4192 | C | ILE | 443 | 108.619 | 30.6722 | 52.283 | 1.00 | 34.90 |
| | 4193 | O | ILE | 443 | 108.866 | 30.908 | 53.469 | 1.00 | 33.18 |
| | 4194 | CB | ILE | 443 | 110.134 | 29.150 | 50.955 | 1.00 | 34.36 |
| | 4195 | CG1 | ILE | 443 | 110.394 | 27.689 | 50.574 | 1.00 | 27.67 |
| 45 | 4196 | CG2 | ILE | 443 | 111.290 | 29.649 | 51.822 | 1.00 | 28.68 |
| | 4197 | CD1 | ILE | 443 | 110.456 | 26.745 | 51.765 | 1.00 | 31.24 |
| | 4198 | H | ILE | 443 | 107.746 | 28.891 | 49.910 | 1.00 | 25.00 |
| | 4199 | N | ASP | 444 | 108.170 | 31.599 | 51.441 | 1.00 | 33.84 |
| | 4200 | CA | ASP | 444 | 107.954 | 32.968 | 51.889 | 1.00 | 35.72 |
| 50 | 4201 | C | ASP | 444 | 106.935 | 32.959 | 53.023 | 1.00 | 38.14 |
| | 4202 | O | ASP | 444 | 107.184 | 33.520 | 54.091 | 1.00 | 37.60 |
| | 4203 | CB | ASP | 444 | 107.450 | 33.848 | 50.744 | 1.00 | 39.61 |

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|----|------|------|-----|-----|----------|--------|--------|------|-------|
| | 4204 | CG | ASP | 444 | 107.110 | 35.260 | 51.199 | 1.00 | 48.15 |
| | 4205 | OD11 | ASP | 444 | 105.972 | 35.485 | 51.667 | 1.00 | 51.59 |
| | 4206 | OD2 | ASP | 444 | 107.980 | 36.147 | 51.091 | 1.00 | 51.59 |
| | 4207 | H | ASP | 444 | 107.985 | 31.364 | 50.507 | 1.00 | 25.00 |
| 5 | 4208 | N | ASP | 445 | 105.812 | 32.279 | 52.803 | 1.00 | 40.33 |
| | 4209 | CA | ASP | 445 | 104.749 | 32.199 | 53.803 | 1.00 | 39.63 |
| | 4210 | C | ASP | 445 | 105.221 | 31.599 | 55.124 | 1.00 | 36.43 |
| | 4211 | O | ASP | 445 | 104.826 | 32.060 | 56.195 | 1.00 | 38.68 |
| | 4212 | CB | ASP | 445 | 103.549 | 31.415 | 53.259 | 1.00 | 34.74 |
| 10 | 4213 | CG | ASP | 445 | 102.867 | 32.115 | 52.087 | 1.00 | 37.47 |
| | 4214 | OD1 | ASP | 445 | 103.173 | 33.301 | 51.818 | 1.00 | 32.84 |
| | 4215 | OD2 | ASP | 445 | 102.022 | 31.474 | 51.429 | 1.00 | 34.75 |
| | 4216 | H | ASP | 445 | 105.694 | 31.823 | 51.945 | 1.00 | 25.00 |
| | 4217 | N | THR | 446 | 106.061 | 30.574 | 55.047 | 1.00 | 36.21 |
| 15 | 4218 | CA | THR | 446 | 106.586 | 29.933 | 56.247 | 1.00 | 34.20 |
| | 4219 | C | THR | 446 | 107.469 | 30.902 | 57.034 | 1.00 | 34.56 |
| | 4220 | O | THR | 446 | 107.396 | 30.968 | 58.259 | 1.00 | 36.69 |
| | 4221 | CB | THR | 446 | 107.398 | 28.674 | 55.890 | 1.00 | 29.80 |
| | 4222 | OG1 | THR | 446 | 106.545 | 27.735 | 55.227 | 1.00 | 31.60 |
| 20 | 4223 | CG2 | THR | 446 | 107.970 | 28.029 | 57.136 | 1.00 | 31.33 |
| | 4224 | H | THR | 446 | 106.322 | 30.221 | 54.170 | 1.00 | 25.00 |
| | 4225 | HG1 | THR | 446 | 107.041 | 26.946 | 54.992 | 1.00 | 25.00 |
| | 4226 | N | ALA | 447 | 108.266 | 31.687 | 56.318 | 1.00 | 39.84 |
| | 4227 | CA | ALA | 447 | 109.172 | 32.644 | 56.941 | 1.00 | 42.07 |
| 25 | 4228 | C | ALA | 447 | 108.495 | 33.902 | 57.483 | 1.00 | 45.04 |
| | 4229 | O | ALA | 447 | 108.675 | 34.259 | 58.647 | 1.00 | 48.71 |
| | 4230 | CB | ALA | 447 | 110.2776 | 33.025 | 55.959 | 1.00 | 36.91 |
| | 4231 | H | ALA | 447 | 108.237 | 31.624 | 55.337 | 1.00 | 25.00 |
| | 4232 | N | THR | 448 | 107.708 | 34.565 | 56.644 | 1.00 | 50.59 |
| 30 | 4233 | CA | THR | 448 | 107.036 | 35.799 | 57.039 | 1.00 | 49.97 |
| | 4234 | C | THR | 448 | 105.729 | 35.644 | 57.818 | 1.00 | 51.43 |
| | 4235 | O | THR | 448 | 105.100 | 36.646 | 58.159 | 1.00 | 56.61 |
| | 4236 | CB | THR | 448 | 106.790 | 36.715 | 55.811 | 1.00 | 47.11 |
| | 4237 | OG1 | THR | 448 | 106.095 | 35.986 | 54.793 | 1.00 | 50.09 |
| 35 | 4238 | CG2 | THR | 448 | 108.106 | 37.214 | 55.245 | 1.00 | 47.36 |
| | 4239 | H | THR | 448 | 107.555 | 34.230 | 55.741 | 1.00 | 25.00 |
| | 4240 | HG1 | THR | 448 | 105.951 | 36.556 | 54.034 | 1.00 | 25.00 |
| | 4241 | N | TYR | 449 | 105.352 | 34.415 | 58.157 | 1.00 | 51.91 |
| | 4242 | CA | TYR | 449 | 104.103 | 34.182 | 58.881 | 1.00 | 53.63 |
| 40 | 4243 | C | TYR | 449 | 103.927 | 35.020 | 60.148 | 1.00 | 58.13 |
| | 4244 | O | TYR | 449 | 102.939 | 35.745 | 60.282 | 1.00 | 57.88 |
| | 4245 | CB | TYR | 449 | 103.926 | 32.696 | 59.218 | 1.00 | 50.75 |
| | 4246 | CG | TYR | 449 | 102.674 | 32.406 | 60.025 | 1.00 | 55.96 |
| | 4247 | CD1 | TYR | 449 | 101.419 | 32.856 | 59.596 | 1.00 | 60.14 |
| 45 | 4248 | CD2 | TYR | 449 | 102.746 | 31.716 | 61.235 | 1.00 | 56.00 |
| | 4249 | CE1 | TYR | 449 | 100.273 | 32.629 | 60.353 | 1.00 | 55.79 |
| | 4250 | CE2 | TYR | 449 | 101.605 | 31.483 | 62.000 | 1.00 | 57.85 |
| | 4251 | CZ | TYR | 449 | 100.375 | 31.943 | 61.554 | 1.00 | 60.06 |
| | 4252 | OH | TYR | 449 | 99.250 | 31.724 | 62.316 | 1.00 | 61.67 |
| 50 | 4253 | H | TYR | 449 | 105.912 | 33.653 | 57.905 | 1.00 | 25.00 |
| | 4254 | HH | TYR | 449 | 98.487 | 32.104 | 61.878 | 1.00 | 25.00 |
| | 4255 | N | GLU | 450 | 104.883 | 34.927 | 61.067 | 1.00 | 64.21 |

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|----|------|-----|------|-----|---------|--------|---------|------|--------|
| | 4256 | CA | GLU | 450 | 104.810 | 35.662 | 62.329 | 1.00 | 67.19 |
| | 4257 | C | GLU | 450 | 104.604 | 37.167 | 62.173 | 1.00 | 68.02 |
| | 4258 | O | GLU | 450 | 103.698 | 37.742 | 62.781 | 1.00 | 68.60 |
| | 4259 | CB | GLU | 450 | 106.053 | 35.386 | 63.178 | 1.00 | 73.69 |
| 5 | 4260 | CG | GLU | 450 | 106.228 | 33.917 | 63.557 | 1.00 | 87.48 |
| | 4261 | CD | GLU | 450 | 104.988 | 33.311 | 64.211 | 1.00 | 95.20 |
| | 4262 | OE1 | GLU | 450 | 104.311 | 34.009 | 65.000 | 1.00 | 100.27 |
| | 4263 | OE2 | GLU | 450 | 104.690 | 32.129 | 63.934 | 1.00 | 96.38 |
| | 4264 | H | GLU | 450 | 105.651 | 34.348 | 60.883 | 1.00 | 25.00 |
| 10 | 4265 | N | VAL | 451 | 105.427 | 37.790 | 61.336 | 1.00 | 69.29 |
| | 4266 | CA | VAL | 451 | 105.351 | 39.228 | 61.091 | 1.00 | 69.79 |
| | 4267 | C | VAL | 451 | 104.011 | 39.634 | 60.479 | 1.00 | 71.86 |
| | 4268 | O | VAL | 451 | 103.383 | 40.594 | 60.925 | 1.00 | 73.87 |
| | 4269 | CB | VAL | 451 | 106.482 | 39.692 | 60.149 | 1.00 | 68.77 |
| 15 | 4270 | CG1 | VAL | 451 | 106.490 | 41.211 | 60.036 | 1.00 | 67.70 |
| | 4271 | CG2 | VAL | 451 | 107.825 | 39.180 | 60.647 | 1.00 | 74.55 |
| | 4272 | H | VAL | 451 | 106.100 | 37.263 | 60.866 | 1.00 | 25.00 |
| | 4273 | N | GLU | 452 | 103.572 | 38.893 | 59.467 | 1.00 | 73.34 |
| | 4274 | CA | GLU | 452 | 102.311 | 39.191 | 58.798 | 1.00 | 74.52 |
| 20 | 4275 | C | GLU | 452 | 101.096 | 38.987 | 59.700 | 1.00 | 75.62 |
| | 4276 | O | GLU | 452 | 100.107 | 39.715 | 59.575 | 1.00 | 75.03 |
| | 4277 | CB | GLU | 452 | 102.176 | 38.385 | 57.502 | 1.00 | 73.01 |
| | 4278 | CG | GLU | 452 | 103.194 | 38.774 | 56.427 | 1.00 | 77.67 |
| | 4279 | CD | GLU | 452 | 103.032 | 38.007 | 55.118 | 1.00 | 81.85 |
| 25 | 4280 | OE1 | GLU | 452 | 102.537 | 36.858 | 55.137 | 1.00 | 80.20 |
| | 4281 | OE2 | GLU | 452 | 103.417 | 38.558 | 54.061 | 1.00 | 82.09 |
| | 4282 | H | GLU | 452 | 104.100 | 38.124 | 59.165 | 1.00 | 25.00 |
| | 4283 | N | LYS | 453 | 101.173 | 38.038 | 60.631 | 1.00 | 78.11 |
| | 4284 | CA | LYS | 453 | 100.050 | 37.799 | 61.536 | 1.00 | 81.43 |
| 30 | 4285 | C | LYS | 453 | 99.887 | 38.943 | 62.532 | 1.00 | 84.49 |
| | 4286 | O | LYS | 453 | 98.768 | 39.393 | 62.783 | 1.00 | 88.82 |
| | 4287 | CB | LYS | 453 | 100.176 | 36.468 | 62.280 | 1.00 | 79.17 |
| | 4288 | CG | LYS | 453 | 98.907 | 36.134 | 63.054 | 1.00 | 78.09 |
| | 4289 | CD | LYS | 453 | 98.928 | 34.759 | 63.674 | 1.00 | 79.02 |
| 35 | 4290 | CE | LYS | 453 | 97.583 | 34.462 | 64.319 | 1.00 | 81.56 |
| | 4291 | NZ | LYS | 453 | 97.525 | 33.093 | 64.899 | 1.00 | 87.65 |
| | 4292 | H | LYS | 453 | 101.981 | 37.486 | 60.701 | 1.00 | 25.00 |
| | 4293 | 1HZ | LYS | 453 | 98.261 | 32.991 | 665.627 | 1.00 | 25.00 |
| | 4294 | 2HZ | LYS | 453 | 96.590 | 32.937 | 65.327 | 1.00 | 25.00 |
| 40 | 4295 | 3HZ | LYS | 453 | 97.682 | 32.390 | 64.148 | 1.00 | 25.00 |
| | 4296 | N | SER | 454 | 100.996 | 39.424 | 63.088 | 1.00 | 84.86 |
| | 4297 | CA | SER | 454 | 100.943 | 40.535 | 64.037 | 1.00 | 83.61 |
| | 4298 | C | SER | 454 | 100.521 | 41.835 | 63.336 | 1.00 | 83.52 |
| | 4299 | O | SER | 454 | 100.210 | 42.830 | 63.991 | 1.00 | 82.37 |
| 45 | 4300 | CB | SER | 454 | 102.286 | 40.703 | 64.755 | 1.00 | 81.64 |
| | 4301 | OG | SER | 454 | 103.363 | 40.771 | 63.838 | 1.00 | 82.19 |
| | 4302 | H | SER | 454 | 101.863 | 39.025 | 62.862 | 1.00 | 25.00 |
| | 4303 | HG | SER | 454 | 103.411 | 39.963 | 63.320 | 1.00 | 25.00 |
| | 4304 | N | ARG | 455 | 100.515 | 41.813 | 62.003 | 1.00 | 83.63 |
| 50 | 4305 | CA | ARG | 455 | 100.102 | 42.961 | 61.197 | 1.00 | 86.97 |
| | 4306 | C | ARRG | 455 | 98.616 | 42.870 | 60.854 | 1.00 | 89.33 |
| | 4307 | O | ARG | 455 | 98.073 | 43.748 | 60.183 | 1.00 | 89.55 |

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|----|------|------|-----|-----|---------|--------|--------|------|--------|
| | 4308 | CB | ARG | 455 | 100.892 | 43.025 | 59.891 | 1.00 | 86.51 |
| | 4309 | CG | ARG | 455 | 102.319 | 43.493 | 60.014 | 1.00 | 89.64 |
| | 4310 | CD | ARG | 455 | 102.926 | 43.581 | 58.632 | 1.00 | 98.07 |
| | 4311 | NE | ARG | 455 | 104.296 | 44.078 | 58.647 | 1.00 | 109.66 |
| 5 | 4312 | CZ | ARG | 455 | 104.976 | 44.415 | 57.555 | 1.00 | 114.68 |
| | 4313 | NH1 | ARG | 455 | 104.411 | 44.309 | 56.357 | 1.00 | 117.44 |
| | 4314 | NH2 | ARG | 455 | 106.220 | 44.863 | 57.659 | 1.00 | 113.39 |
| | 4315 | H | ARG | 455 | 100.816 | 41.007 | 61.542 | 1.00 | 25.00 |
| | 4316 | HE | ARG | 455 | 104.745 | 44.172 | 59.512 | 1.00 | 25.00 |
| 10 | 4317 | 1HH1 | ARG | 455 | 103.471 | 43.978 | 56.270 | 1.00 | 25.00 |
| | 4318 | 2HH1 | ARG | 455 | 104.920 | 44.568 | 55.536 | 1.00 | 25.00 |
| | 4319 | 1HH2 | ARG | 455 | 106.646 | 44.949 | 58.558 | 1.00 | 25.00 |
| | 4320 | 2HH2 | ARG | 455 | 105.724 | 45.120 | 56.834 | 1.00 | 25.00 |
| | 4321 | N | GLY | 456 | 97.980 | 41.773 | 61.259 | 1.00 | 90.67 |
| 15 | 4322 | CA | GLY | 456 | 96.566 | 41.584 | 60.989 | 1.00 | 90.27 |
| | 4323 | C | GLY | 456 | 96.256 | 40.876 | 59.681 | 1.00 | 91.84 |
| | 4324 | O | GLY | 456 | 95.087 | 40.636 | 59.371 | 1.00 | 90.99 |
| | 4325 | H | GLY | 456 | 98.464 | 41.081 | 61.752 | 1.00 | 25.00 |
| | 4326 | N | GLN | 457 | 97.290 | 40.528 | 58.917 | 1.00 | 92.16 |
| 20 | 4327 | CA | GLN | 457 | 97.107 | 39.842 | 57.638 | 1.00 | 90.85 |
| | 4328 | C | GLN | 457 | 96.662 | 38.395 | 57.846 | 1.00 | 89.74 |
| | 4329 | O | GLN | 457 | 97.442 | 37.462 | 57.659 | 1.00 | 92.66 |
| | 4330 | CB | GLN | 457 | 98.402 | 39.868 | 56.817 | 1.00 | 89.90 |
| | 4331 | CG | GLN | 457 | 98.905 | 41.257 | 56.457 | 1.00 | 95.19 |
| 25 | 4332 | CD | GLN | 457 | 100.145 | 41.221 | 55.576 | 1.00 | 99.21 |
| | 4333 | OE1 | GLN | 457 | 100.325 | 40.303 | 54.775 | 1.00 | 102.27 |
| | 4334 | NE2 | GLN | 457 | 101.002 | 42.225 | 55.718 | 1.00 | 97.71 |
| | 4335 | H | GLN | 457 | 98.199 | 40.716 | 59.228 | 1.00 | 25.00 |
| | 4336 | 1HE2 | GLN | 457 | 101.798 | 42.200 | 55.151 | 1.00 | 25.00 |
| 30 | 4337 | 2HE2 | GLN | 457 | 100.809 | 42.931 | 56.364 | 1.00 | 25.00 |
| | 4338 | N | ILE | 458 | 95.397 | 38.207 | 58.209 | 1.00 | 88.19 |
| | 4339 | CA | ILE | 458 | 94.859 | 36.867 | 58.439 | 1.00 | 82.29 |
| | 4340 | C | ILE | 458 | 94.715 | 36.043 | 57.159 | 1.00 | 75.34 |
| | 4341 | O | ILE | 458 | 94.305 | 34.887 | 57.205 | 1.00 | 73.69 |
| 35 | 4342 | CB | ILE | 458 | 93.510 | 36.907 | 59.199 | 1.00 | 85.78 |
| | 4343 | CG1 | ILE | 458 | 92.566 | 37.933 | 58.562 | 1.00 | 86.17 |
| | 4344 | CG2 | ILE | 458 | 93.751 | 37.191 | 60.681 | 1.00 | 85.33 |
| | 4345 | CD1 | ILE | 458 | 91.240 | 38.069 | 59.277 | 1.00 | 89.41 |
| | 4346 | H | ILE | 458 | 94.823 | 38.995 | 58.338 | 1.00 | 25.00 |
| 40 | 4347 | N | ALA | 459 | 95.077 | 36.632 | 56.025 | 1.00 | 68.80 |
| | 4348 | CA | ALA | 459 | 95.007 | 35.936 | 54.747 | 1.00 | 62.63 |
| | 4349 | C | ALA | 459 | 96.368 | 35.324 | 54.389 | 1.00 | 62.33 |
| | 4350 | O | ALA | 459 | 96.664 | 35.093 | 53.216 | 1.00 | 62.33 |
| | 4351 | CB | ALA | 459 | 94.549 | 36.893 | 53.653 | 1.00 | 62.28 |
| 45 | 4352 | H | ALA | 459 | 95.387 | 37.554 | 56.036 | 1.00 | 25.00 |
| | 4353 | N | THR | 460 | 97.210 | 35.097 | 55.396 | 1.00 | 59.27 |
| | 4354 | CA | THR | 460 | 98.531 | 34.513 | 55.170 | 1.00 | 57.11 |
| | 4355 | C | THR | 460 | 98.424 | 33.034 | 54.826 | 1.00 | 53.62 |
| | 4356 | O | THR | 460 | 97.587 | 32.319 | 55.383 | 1.00 | 53.81 |
| 50 | 4357 | CB | THR | 460 | 99.453 | 34.671 | 56.400 | 1.00 | 58.87 |
| | 4358 | OG1 | THR | 460 | 98.763 | 34.257 | 57.588 | 1.00 | 56.81 |
| | 4359 | CG2 | THR | 460 | 99.901 | 36.100 | 56.541 | 1.00 | 60.73 |

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|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 4360 | H | THR | 460 | 96.933 | 35.314 | 56.305 | 1.00 | 25.00 |
| | 4361 | HG1 | THR | 460 | 98.004 | 34.838 | 57.727 | 1.00 | 25.00 |
| | 4362 | N | GLY | 461 | 99.298 | 32.574 | 53.937 | 1.00 | 44.28 |
| | 4363 | CA | GLY | 461 | 99.289 | 31.184 | 53.526 | 1.00 | 37.76 |
| 5 | 4364 | C | GLY | 461 | 99.138 | 30.186 | 54.652 | 1.00 | 39.21 |
| | 4365 | O | GLY | 461 | 98.265 | 29.318 | 54.599 | 1.00 | 37.71 |
| | 4366 | H | GLY | 461 | 99.947 | 33.183 | 53.532 | 1.00 | 25.00 |
| | 4367 | N | ILE | 462 | 99.965 | 30.320 | 55.684 | 1.00 | 41.07 |
| | 4368 | CA | ILE | 462 | 99.915 | 29.405 | 56.821 | 1.00 | 43.03 |
| 10 | 4369 | C | ILE | 462 | 98.567 | 29.461 | 57.539 | 1.00 | 43.30 |
| | 4370 | O | ILE | 462 | 98.063 | 28.430 | 57.991 | 1.00 | 44.23 |
| | 4371 | CB | ILE | 462 | 101.079 | 29.658 | 57.814 | 1.00 | 35.94 |
| | 4372 | CG1 | ILE | 462 | 102.418 | 29.419 | 57.116 | 1.00 | 34.23 |
| | 4373 | CG2 | ILE | 462 | 100.979 | 28.720 | 59.011 | 1.00 | 26.77 |
| 15 | 4374 | CD1 | ILE | 462 | 102.625 | 27.987 | 56.675 | 1.00 | 31.75 |
| | 4375 | H | ILE | 462 | 100.618 | 31.046 | 55.680 | 1.00 | 25.00 |
| | 4376 | N | GLU | 463 | 97.972 | 30.652 | 57.602 | 1.00 | 47.45 |
| | 4377 | CA | GLU | 463 | 96.673 | 30.842 | 58.253 | 1.00 | 48.26 |
| | 4378 | C | GLU | 463 | 95.600 | 30.064 | 57.495 | 1.00 | 43.95 |
| 20 | 4379 | O | GLU | 463 | 94.876 | 29.250 | 58.077 | 1.00 | 45.29 |
| | 4380 | CB | GLU | 463 | 96.307 | 32.329 | 58.291 | 1.00 | 55.50 |
| | 4381 | CG | GLU | 463 | 95.120 | 32.664 | 59.182 | 1.00 | 60.77 |
| | 4382 | CD | GLU | 463 | 95.448 | 32.555 | 60.656 | 1.00 | 66.36 |
| | 4383 | OE1 | GLU | 463 | 96.195 | 33.419 | 61.166 | 1.00 | 70.77 |
| 25 | 4384 | OE2 | GLU | 463 | 94.957 | 31.605 | 61.303 | 1.00 | 66.97 |
| | 4385 | H | GLU | 463 | 98.403 | 31.430 | 57.193 | 1.00 | 25.00 |
| | 4386 | N | CYS | 464 | 95.534 | 30.295 | 56.186 | 1.00 | 38.49 |
| | 4387 | CA | CYS | 464 | 94.575 | 29.616 | 55.322 | 1.00 | 40.30 |
| | 4388 | C | CYS | 464 | 94.751 | 28.113 | 55.451 | 1.00 | 40.72 |
| 30 | 4389 | O | CYS | 464 | 93.778 | 27.364 | 55.550 | 1.00 | 43.89 |
| | 4390 | CB | CYS | 464 | 94.798 | 30.010 | 53.860 | 1.00 | 33.19 |
| | 4391 | SG | CYS | 464 | 94.721 | 31.780 | 53.533 | 1.00 | 41.13 |
| | 4392 | H | CYS | 464 | 96.143 | 30.954 | 55.789 | 1.00 | 25.00 |
| | 4393 | N | CYS | 465 | 96.007 | 27.682 | 55.464 | 1.00 | 42.83 |
| 35 | 4394 | CA | CYS | 465 | 96.337 | 26.271 | 55.557 | 1.00 | 45.44 |
| | 4395 | C | CYS | 465 | 95.791 | 25.654 | 56.852 | 1.00 | 48.27 |
| | 4396 | O | CYS | 465 | 95.165 | 24.591 | 56.818 | 1.00 | 47.36 |
| | 4397 | CB | CYS | 465 | 97.850 | 26.074 | 55.487 | 1.00 | 39.55 |
| | 4398 | SG | CYS | 465 | 98.332 | 24.350 | 55.349 | 1.00 | 40.18 |
| 40 | 4399 | H | CYS | 465 | 96.735 | 28.334 | 55.396 | 1.00 | 25.00 |
| | 4400 | N | MET | 466 | 96.000 | 26.340 | 57.972 | 1.00 | 51.35 |
| | 4401 | CA | MET | 466 | 95.531 | 25.854 | 59.267 | 1.00 | 55.36 |
| | 4402 | C | MET | 466 | 94.019 | 25.699 | 59.312 | 1.00 | 56.30 |
| | 4403 | O | MET | 466 | 93.512 | 24.647 | 59.698 | 1.00 | 55.90 |
| 45 | 4404 | CB | MET | 466 | 95.977 | 26.786 | 60.391 | 1.00 | 52.93 |
| | 4405 | CG | MET | 466 | 97.464 | 26.797 | 60.618 | 1.00 | 49.91 |
| | 4406 | SD | MET | 466 | 97.890 | 27.866 | 61.980 | 1.00 | 56.57 |
| | 4407 | CE | MET | 466 | 97.679 | 29.434 | 61.228 | 1.00 | 45.63 |
| | 4408 | H | MET | 466 | 96.483 | 27.193 | 57.936 | 1.00 | 25.00 |
| 50 | 4409 | N | ARG | 467 | 93.303 | 26.744 | 58.916 | 1.00 | 57.72 |
| | 4410 | CA | ARG | 467 | 91.849 | 26.704 | 58.921 | 1.00 | 60.99 |
| | 4411 | C | ARG | 467 | 91.271 | 25.700 | 57.935 | 1.00 | 57.48 |

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|----|------|------|-----|-----|--------|--------|--------|------|--------|
| | 4412 | O | ARG | 467 | 90.406 | 24.901 | 58.295 | 1.00 | 61.64 |
| | 4413 | CB | ARG | 467 | 91.270 | 28.089 | 58.642 | 1.00 | 69.59 |
| | 4414 | CG | ARG | 467 | 91.304 | 29.011 | 59.839 | 1.00 | 84.26 |
| | 4415 | CD | ARG | 467 | 90.397 | 30.202 | 59.616 | 1.00 | 96.57 |
| 5 | 4416 | NE | ARG | 467 | 90.163 | 30.938 | 60.853 | 1.00 | 103.82 |
| | 4417 | CZ | ARG | 467 | 89.074 | 31.660 | 61.099 | 1.00 | 107.61 |
| | 4418 | NH1 | ARG | 467 | 88.109 | 31.749 | 60.192 | 1.00 | 108.04 |
| | 4419 | NH2 | ARG | 467 | 88.946 | 32.284 | 62.261 | 1.00 | 109.38 |
| | 4420 | H | ARG | 467 | 93.769 | 27.556 | 58.623 | 1.00 | 25.00 |
| 10 | 4421 | HE | ARG | 467 | 90.848 | 30.890 | 61.554 | 1.00 | 25.00 |
| | 4422 | 1HH1 | ARG | 467 | 88.194 | 31.273 | 59.318 | 1.00 | 25.00 |
| | 4423 | 2HH1 | ARG | 467 | 87.293 | 32.293 | 60.390 | 1.00 | 25.00 |
| | 4424 | 1HH2 | ARG | 467 | 89.669 | 32.209 | 62.950 | 1.00 | 25.00 |
| | 4425 | 2HH2 | ARG | 467 | 88.130 | 32.827 | 62.457 | 1.00 | 25.00 |
| 15 | 4426 | N | ASP | 468 | 91.769 | 25.726 | 56.704 | 1.00 | 52.60 |
| | 4427 | CA | ASP | 468 | 91.287 | 24.832 | 55.660 | 1.00 | 51.80 |
| | 4428 | C | ASP | 468 | 91.404 | 23.354 | 56.032 | 1.00 | 52.54 |
| | 4429 | O | ASP | 468 | 90.488 | 22.574 | 55.767 | 1.00 | 57.49 |
| | 4430 | CB | ASP | 468 | 92.026 | 25.111 | 54.346 | 1.00 | 49.09 |
| 20 | 4431 | CG | ASP | 468 | 91.328 | 24.513 | 53.133 | 1.00 | 52.94 |
| | 4432 | OD1 | ASP | 468 | 90.127 | 24.170 | 53.218 | 1.00 | 55.18 |
| | 4433 | OD2 | ASP | 468 | 91.983 | 24.402 | 52.076 | 1.00 | 54.77 |
| | 4434 | H | ASP | 468 | 92.480 | 26.362 | 56.496 | 1.00 | 25.00 |
| | 4435 | N | TYR | 469 | 92.524 | 22.973 | 56.646 | 1.00 | 52.44 |
| 25 | 4436 | CA | TYR | 469 | 92.755 | 21.581 | 57.040 | 1.00 | 49.37 |
| | 4437 | C | TYR | 469 | 92.458 | 21.283 | 58.511 | 1.00 | 48.25 |
| | 4438 | O | TYR | 469 | 92.316 | 20.121 | 58.894 | 1.00 | 46.98 |
| | 4439 | CB | TYR | 469 | 94.200 | 21.165 | 56.730 | 1.00 | 46.99 |
| | 4440 | CG | TYR | 469 | 94.546 | 21.129 | 55.260 | 1.00 | 47.76 |
| 30 | 4441 | CD1 | TYR | 469 | 94.994 | 22.273 | 54.602 | 1.00 | 51.80 |
| | 4442 | CD2 | TYR | 469 | 94.431 | 19.947 | 54.524 | 1.00 | 50.13 |
| | 4443 | CE1 | TYR | 469 | 95.317 | 22.246 | 53.248 | 1.00 | 56.40 |
| | 4444 | CE2 | TYR | 469 | 94.753 | 19.908 | 53.167 | 1.00 | 54.09 |
| | 4445 | CZ | TYR | 469 | 95.195 | 21.063 | 52.537 | 1.00 | 57.04 |
| 35 | 4446 | OH | TYR | 469 | 95.514 | 21.044 | 51.198 | 1.00 | 62.08 |
| | 4447 | H | TYR | 469 | 93.216 | 23.642 | 56.837 | 1.00 | 25.00 |
| | 4448 | HH | TYR | 469 | 95.802 | 21.916 | 50.922 | 1.00 | 25.00 |
| | 4449 | N | GLY | 470 | 92.371 | 22.328 | 59.328 | 1.00 | 49.37 |
| | 4450 | CA | GLY | 470 | 92.113 | 22.147 | 60.746 | 1.00 | 51.47 |
| 40 | 4451 | C | GLY | 470 | 93.332 | 21.551 | 61.425 | 1.00 | 52.90 |
| | 4452 | O | GLY | 470 | 93.247 | 20.499 | 62.064 | 1.00 | 54.39 |
| | 4453 | H | GLY | 470 | 92.471 | 23.228 | 58.968 | 1.00 | 25.00 |
| | 4454 | N | ILE | 471 | 94.467 | 22.238 | 61.300 | 1.00 | 53.10 |
| | 4455 | CA | ILE | 471 | 95.728 | 21.771 | 61.874 | 1.00 | 48.51 |
| 45 | 4456 | C | ILE | 471 | 96.521 | 22.877 | 62.571 | 1.00 | 49.16 |
| | 4457 | O | ILE | 471 | 96.230 | 24.063 | 62.408 | 1.00 | 48.02 |
| | 4458 | CB | ILE | 471 | 96.617 | 21.131 | 60.781 | 1.00 | 44.19 |
| | 4459 | CG1 | ILE | 471 | 96.816 | 22.116 | 59.621 | 1.00 | 43.37 |
| | 4460 | CG2 | ILE | 471 | 95.991 | 19.829 | 60.288 | 1.00 | 41.20 |
| 50 | 4461 | CD1 | ILE | 471 | 97.608 | 21.558 | 58.449 | 1.00 | 38.24 |
| | 4462 | H | ILE | 471 | 94.452 | 23.094 | 60.822 | 1.00 | 25.00 |
| | 4463 | N | SER | 472 | 97.517 | 22.475 | 63.357 | 1.00 | 53.02 |

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|----|------|-----|-----|------|---------|--------|--------|------|-------|
| | 4464 | CA | SER | 472 | 98.371 | 23.414 | 64.085 | 1.00 | 57.32 |
| | 4465 | C | SER | 472 | 99.352 | 24.117 | 63.146 | 1.00 | 60.76 |
| | 4466 | O | SER | 472 | 99.689 | 23.587 | 62.084 | 1.00 | 61.94 |
| | 4467 | CB | SER | 472 | 99.148 | 22.672 | 65.180 | 1.00 | 59.87 |
| 5 | 4468 | OG | SER | 472 | 99.873 | 21.568 | 64.653 | 1.00 | 59.66 |
| | 4469 | H | SER | 472 | 97.697 | 21.518 | 63.453 | 1.00 | 25.00 |
| | 4470 | HG | SER | 472 | 100.314 | 21.103 | 65.376 | 1.00 | 25.00 |
| | 4471 | N | THR | 473 | 99.838 | 25.287 | 63.557 | 1.00 | 61.86 |
| | 4472 | CA | THR | 473 | 100.794 | 26.053 | 62.755 | 1.00 | 63.28 |
| 10 | 4473 | C | THR | 473 | 101.959 | 25.160 | 62.340 | 1.00 | 66.44 |
| | 4474 | O | THR | 473 | 102.374 | 25.158 | 61.179 | 1.00 | 66.96 |
| | 4475 | CB | THR | 473 | 101.366 | 27.248 | 63.547 | 1.00 | 62.70 |
| | 4476 | OG1 | THR | 473 | 100.295 | 28.083 | 63.997 | 1.00 | 63.68 |
| | 4477 | CG2 | THR | 473 | 102.306 | 28.068 | 62.677 | 1.00 | 63.27 |
| 15 | 4478 | H | THR | 473 | 99.529 | 25.654 | 64.404 | 1.00 | 25.00 |
| | 4479 | HG1 | THR | 473 | 99.682 | 27.608 | 64.552 | 1.00 | 25.00 |
| | 4480 | N | LYS | 474 | 102.454 | 24.380 | 63.296 | 1.00 | 65.27 |
| | 4481 | CA | LYS | 474 | 103.568 | 23.470 | 63.065 | 1.00 | 67.87 |
| | 4482 | C | LYS | 474 | 103.248 | 22.508 | 61.922 | 1.00 | 65.57 |
| 20 | 4483 | O | LYS | 474 | 104.051 | 22.325 | 61.001 | 1.00 | 66.11 |
| | 4484 | CB | LYS | 474 | 103.863 | 22.686 | 64.349 | 1.00 | 71.33 |
| | 4485 | CG | LYS | 474 | 105.150 | 21.875 | 64.320 | 1.00 | 77.07 |
| | 4486 | CD | LYS | 474 | 105.422 | 21.234 | 65.673 | 1.00 | 77.42 |
| | 4487 | CE | LYS | 474 | 106.776 | 20.544 | 65.698 | 1.00 | 78.55 |
| 25 | 4488 | NZ | LYS | 474 | 107.067 | 19.962 | 67.037 | 1.00 | 75.57 |
| | 4489 | H | LYS | 474 | 102.058 | 24.422 | 64.186 | 1.00 | 25.00 |
| | 4490 | 1HZ | LYS | 474 | 106.336 | 19.263 | 67.278 | 1.00 | 25.00 |
| | 4491 | 2HZ | LYS | 474 | 107.998 | 19.500 | 67.020 | 1.00 | 25.00 |
| | 4492 | 3HZ | LYS | 474 | 107.070 | 20.720 | 67.750 | 1.00 | 25.00 |
| 30 | 4493 | N | GLU | 475 | 102.047 | 21.944 | 61.960 | 1.00 | 61.44 |
| | 4494 | CA | GLU | 475 | 101.612 | 20.998 | 60.945 | 1.00 | 57.77 |
| | 4495 | C | GLU | 475 | 101.378 | 21.683 | 59.599 | 1.00 | 53.01 |
| | 4496 | O | GLU | 475 | 101.623 | 21.091 | 58.545 | 1.00 | 55.03 |
| | 4497 | CB | GLU | 475 | 100.352 | 20.282 | 61.418 | 1.00 | 59.71 |
| 35 | 4498 | CG | GLU | 475 | 100.104 | 18.950 | 60.737 | 1.00 | 73.81 |
| | 4499 | CD | GLU | 475 | 98.994 | 18.148 | 61.399 | 1.00 | 84.47 |
| | 4500 | OE1 | GLU | 475 | 98.562 | 18.513 | 62.518 | 1.00 | 88.32 |
| | 4501 | OE2 | GLU | 475 | 98.555 | 17.144 | 60.797 | 1.00 | 88.90 |
| | 4502 | H | GLU | 475 | 101.423 | 22.181 | 62.675 | 1.00 | 25.00 |
| 40 | 4503 | N | ALA | 476 | 100.931 | 22.936 | 59.637 | 1.00 | 46.25 |
| | 4504 | CA | ALA | 476 | 100.681 | 23.703 | 58.420 | 1.00 | 43.91 |
| | 4505 | C | ALA | 476 | 102.003 | 23.972 | 57.712 | 1.00 | 44.05 |
| | 4506 | O | ALA | 476 | 102.124 | 23.774 | 56.501 | 1.00 | 42.50 |
| | 4507 | CB | ALA | 476 | 99.984 | 25.018 | 58.749 | 1.00 | 34.16 |
| 45 | 4508 | H | ALA | 4776 | 100.761 | 23.358 | 60.501 | 1.00 | 25.00 |
| | 4509 | N | MET | 477 | 103.000 | 24.402 | 58.480 | 1.00 | 45.42 |
| | 4510 | CA | MET | 477 | 104.321 | 24.689 | 57.932 | 1.00 | 46.57 |
| | 4511 | C | MET | 477 | 104.954 | 23.414 | 57.395 | 1.00 | 46.73 |
| | 4512 | O | MET | 477 | 105.640 | 23.434 | 56.369 | 1.00 | 48.81 |
| 50 | 4513 | CB | MET | 477 | 105.217 | 25.331 | 58.990 | 1.00 | 41.20 |
| | 4514 | CG | MET | 477 | 104.699 | 26.674 | 59.459 | 1.00 | 45.53 |
| | 4515 | SD | MET | 477 | 105.842 | 27.539 | 60.529 | 1.00 | 50.24 |

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|----|------|------|-----|-----|---------|---------|--------|------|-------|
| | 4516 | CE | MET | 477 | 105.403 | 29.229 | 60.204 | 1.00 | 44.87 |
| | 4517 | H | MET | 477 | 102.838 | 24.531 | 59.436 | 1.00 | 25.00 |
| | 4518 | N | ALA | 478 | 104.689 | 22.301 | 58.071 | 1.00 | 43.88 |
| | 4519 | CA | ALA | 478 | 105.214 | 21.012 | 57.646 | 1.00 | 40.24 |
| 5 | 4520 | C | ALA | 478 | 104.608 | 20.664 | 56.288 | 1.00 | 39.48 |
| | 4521 | O | ALA | 478 | 105.301 | 20.158 | 55.404 | 1.00 | 42.61 |
| | 4522 | CB | ALA | 478 | 104.887 | 19.941 | 58.673 | 1.00 | 38.44 |
| | 4523 | H | ALA | 478 | 104.140 | 22.350 | 58.883 | 1.00 | 25.00 |
| | 4524 | N | LYS | 479 | 103.324 | 20.969 | 56.113 | 1.00 | 37.41 |
| 10 | 4525 | CA | LYS | 479 | 102.642 | 20.700 | 54.850 | 1.00 | 36.91 |
| | 4526 | C | LYS | 479 | 103.214 | 21.598 | 53.754 | 1.00 | 33.62 |
| | 4527 | O | LYS | 479 | 103.408 | 21.164 | 52.616 | 1.00 | 32.37 |
| | 4528 | CB | LYS | 479 | 101.136 | 20.931 | 54.986 | 1.00 | 39.38 |
| | 4529 | CG | LYS | 479 | 100.338 | 20.573 | 53.736 | 1.00 | 46.00 |
| 15 | 4530 | CD | LYS | 479 | 98.850 | 20.797 | 53.947 | 1.00 | 51.63 |
| | 4531 | CE | LYS | 479 | 98.273 | 19.858 | 55.003 | 1.00 | 53.61 |
| | 4532 | NZ | LYS | 479 | 98.180 | 18.451 | 54.525 | 1.00 | 57.01 |
| | 4533 | H | LYS | 479 | 102.820 | 21.3777 | 56.852 | 1.00 | 25.00 |
| | 4534 | 1HZ | LYS | 479 | 99.126 | 18.106 | 54.269 | 1.00 | 25.00 |
| 20 | 4535 | 2HZ | LYS | 479 | 97.776 | 17.853 | 55.274 | 1.00 | 25.00 |
| | 4536 | 3HZ | LYS | 479 | 97.561 | 18.416 | 53.688 | 1.00 | 25.00 |
| | 4537 | N | PHE | 480 | 103.502 | 22.845 | 54.107 | 1.00 | 30.92 |
| | 4538 | CA | PHE | 480 | 104.067 | 23.790 | 53.157 | 1.00 | 31.88 |
| | 4539 | C | PHE | 480 | 105.457 | 23.356 | 52.714 | 1.00 | 34.12 |
| 25 | 4540 | O | PHE | 480 | 105.812 | 23.493 | 51.540 | 1.00 | 37.15 |
| | 4541 | CB | PHE | 480 | 104.107 | 25.198 | 53.749 | 1.00 | 29.35 |
| | 4542 | CG | PHE | 480 | 102.902 | 26.028 | 53.408 | 1.00 | 37.28 |
| | 4543 | CD1 | PHE | 480 | 101.662 | 25.427 | 53.190 | 1.00 | 37.60 |
| | 4544 | CD2 | PHE | 480 | 103.008 | 27.411 | 53.283 | 1.00 | 36.73 |
| 30 | 4545 | CE1 | PHE | 480 | 100.546 | 26.192 | 52.850 | 1.00 | 36.20 |
| | 4546 | CE22 | PHE | 480 | 101.898 | 28.185 | 52.942 | 1.00 | 38.45 |
| | 4547 | CZ | PHE | 480 | 100.665 | 27.574 | 52.726 | 1.00 | 36.96 |
| | 4548 | H | PHE | 480 | 103.315 | 23.138 | 55.024 | 1.00 | 25.00 |
| | 4549 | N | GLN | 481 | 106.238 | 22.810 | 53.641 | 1.00 | 33.79 |
| 35 | 4550 | CA | GLN | 481 | 107.573 | 22.352 | 53.292 | 1.00 | 35.43 |
| | 4551 | C | GLN | 481 | 107.453 | 21.180 | 52.323 | 1.00 | 35.55 |
| | 4552 | O | GLN | 481 | 108.200 | 21.103 | 51.347 | 1.00 | 35.63 |
| | 4553 | CB | GLN | 481 | 108.368 | 21.930 | 54.524 | 1.00 | 46.60 |
| | 4554 | CG | GLN | 481 | 109.844 | 21.688 | 54.210 | 1.00 | 70.92 |
| 40 | 4555 | CD | GLN | 481 | 110.583 | 20.933 | 55.302 | 1.00 | 83.38 |
| | 4556 | OE1 | GLN | 481 | 110.036 | 20.658 | 56.371 | 1.00 | 93.92 |
| | 4557 | NE2 | GLN | 481 | 111.836 | 20.588 | 55.032 | 1.00 | 88.62 |
| | 4558 | H | GLN | 481 | 105.919 | 22.723 | 54.562 | 1.00 | 25.00 |
| | 4559 | 1HE2 | GLN | 481 | 112.316 | 20.105 | 55.735 | 1.00 | 25.00 |
| 45 | 4560 | 2HE2 | GLN | 481 | 112.220 | 20.824 | 54.166 | 1.00 | 25.00 |
| | 4561 | N | ASN | 482 | 106.486 | 20.297 | 52.561 | 1.00 | 33.51 |
| | 4562 | CA | ASN | 482 | 106.272 | 19.146 | 51.682 | 1.00 | 36.28 |
| | 4563 | C | ASN | 482 | 105.950 | 19.606 | 50.267 | 1.00 | 36.07 |
| | 4564 | O | ASN | 482 | 106.380 | 18.989 | 49.288 | 1.00 | 35.83 |
| 50 | 4565 | CB | ASN | 482 | 105.140 | 18.252 | 52.200 | 1.00 | 40.65 |
| | 4566 | CG | ASN | 482 | 105.535 | 17.465 | 53.436 | 1.00 | 54.20 |
| | 4567 | OD1 | ASN | 482 | 106.698 | 17.095 | 53.607 | 1.00 | 57.37 |

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|----|------|------|-----|-----|----------|--------|--------|------|-------|
| | 4568 | ND2 | ASN | 482 | 104.565 | 17.204 | 54.307 | 1.00 | 59.54 |
| | 4569 | H | ASN | 482 | 105.916 | 20.415 | 53.350 | 1.00 | 25.00 |
| | 4570 | 1HD2 | ASN | 482 | 104.821 | 16.698 | 55.105 | 1.00 | 25.00 |
| | 4571 | 2HD2 | ASN | 482 | 103.6661 | 17.519 | 54.121 | 1.00 | 25.00 |
| 5 | 4572 | N | MET | 483 | 105.199 | 20.698 | 50.163 | 1.00 | 33.64 |
| | 4573 | CA | MET | 483 | 104.831 | 21.250 | 48.866 | 1.00 | 29.91 |
| | 4574 | C | MET | 483 | 106.080 | 21.757 | 48.152 | 1.00 | 27.30 |
| | 4575 | O | MET | 483 | 106.240 | 21.556 | 46.947 | 1.00 | 32.31 |
| | 4576 | CB | MET | 483 | 103.814 | 22.373 | 49.036 | 1.00 | 29.58 |
| 10 | 4577 | CG | MET | 483 | 102.488 | 21.916 | 49.626 | 1.00 | 32.65 |
| | 4578 | SD | MET | 483 | 101.388 | 23.311 | 49.943 | 1.00 | 37.42 |
| | 4579 | CE | MET | 483 | 100.988 | 23.770 | 48.275 | 1.00 | 33.87 |
| | 4580 | H | MET | 483 | 104.879 | 21.134 | 50.982 | 1.00 | 25.00 |
| | 4581 | N | ALA | 484 | 106.979 | 22.385 | 48.903 | 1.00 | 24.24 |
| 15 | 4582 | CA | ALA | 484 | 108.226 | 22.895 | 48.339 | 1.00 | 25.37 |
| | 4583 | C | ALA | 484 | 109.086 | 21.724 | 47.845 | 1.00 | 27.23 |
| | 4584 | O | ALA | 484 | 109.696 | 21.792 | 46.772 | 1.00 | 26.13 |
| | 4585 | CB | ALA | 484 | 108.979 | 23.703 | 49.385 | 1.00 | 20.73 |
| | 4586 | H | ALA | 484 | 106.799 | 22.516 | 49.859 | 1.00 | 25.00 |
| 20 | 4587 | N | GLU | 485 | 109.103 | 20.642 | 48.622 | 1.00 | 27.25 |
| | 4588 | CA | GLU | 485 | 109.864 | 19.437 | 48.289 | 1.00 | 29.59 |
| | 4589 | C | GLU | 485 | 109.317 | 18.807 | 47.015 | 1.00 | 26.53 |
| | 4590 | O | GLU | 485 | 110.070 | 18.386 | 46.139 | 1.00 | 32.01 |
| | 4591 | CB | GLU | 485 | 109.792 | 18.425 | 49.437 | 1.00 | 39.77 |
| 25 | 4592 | CG | GLU | 485 | 110.327 | 18.942 | 50.779 | 1.00 | 61.11 |
| | 4593 | CD | GLU | 485 | 110.170 | 17.953 | 51.934 | 1.00 | 69.27 |
| | 4594 | OE1 | GLU | 485 | 109.663 | 16.830 | 51.716 | 1.00 | 73.83 |
| | 4595 | OE2 | GLU | 485 | 110.561 | 18.302 | 53.073 | 1.00 | 69.26 |
| | 4596 | H | GLU | 485 | 108.574 | 20.683 | 49.449 | 1.00 | 25.00 |
| 30 | 4597 | N | THR | 486 | 107.997 | 18.755 | 46.917 | 1.00 | 26.56 |
| | 4598 | CA | THR | 486 | 107.323 | 18.207 | 45.749 | 1.00 | 26.51 |
| | 4599 | C | THR | 486 | 107.673 | 19.050 | 44.520 | 1.00 | 24.78 |
| | 4600 | O | THR | 486 | 107.961 | 18.514 | 43.437 | 1.00 | 24.00 |
| | 4601 | CB | THR | 486 | 105.790 | 18.211 | 45.973 | 1.00 | 30.57 |
| 35 | 4602 | OG1 | THR | 486 | 105.463 | 17.277 | 47.010 | 1.00 | 30.11 |
| | 4603 | CG2 | THR | 486 | 105.034 | 17.855 | 44.694 | 1.00 | 27.79 |
| | 4604 | H | THR | 486 | 107.446 | 19.085 | 47.660 | 1.00 | 25.00 |
| | 4605 | HG1 | THR | 486 | 105.755 | 16.396 | 46.782 | 1.00 | 25.00 |
| | 4606 | N | ALA | 487 | 107.672 | 20.367 | 44.712 | 1.00 | 20.69 |
| 40 | 4607 | CA | ALA | 487 | 107.980 | 21.319 | 43.651 | 1.00 | 19.32 |
| | 4608 | C | ALA | 487 | 109.409 | 21.127 | 43.141 | 1.00 | 18.49 |
| | 4609 | O | ALA | 487 | 109.654 | 21.149 | 41.929 | 1.00 | 15.86 |
| | 4610 | CB | ALA | 487 | 107.768 | 22.750 | 44.152 | 1.00 | 15.08 |
| | 4611 | H | ALA | 487 | 107.454 | 20.716 | 45.604 | 1.00 | 25.00 |
| 45 | 4612 | N | TRP | 488 | 110.349 | 20.909 | 44.058 | 1.00 | 20.11 |
| | 4613 | CA | TRP | 488 | 111.736 | 20.695 | 43.661 | 1.00 | 19.04 |
| | 4614 | C | TRP | 488 | 111.856 | 19.461 | 42.781 | 1.00 | 20.42 |
| | 4615 | O | TRP | 488 | 112.555 | 19.486 | 41.768 | 1.00 | 23.27 |
| | 4616 | CB | TRP | 488 | 112.656 | 20.590 | 44.879 | 1.00 | 19.13 |
| 50 | 4617 | CG | TRP | 488 | 113.256 | 21.905 | 45.262 | 1.00 | 20.79 |
| | 4618 | CD1 | TRP | 488 | 113.017 | 22.619 | 46.402 | 1.00 | 19.35 |
| | 4619 | CD2 | TRP | 488 | 114.173 | 22.689 | 44.481 | 1.00 | 18.53 |

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|----|------|------|------|-----|---------|--------|--------|------|-------|
| | 4620 | NE1 | TRP | 488 | 113.723 | 23.801 | 46.376 | 1.00 | 21.34 |
| | 4621 | CE2 | TRP | 488 | 114.441 | 23.869 | 45.210 | 1.00 | 17.70 |
| | 4622 | CE3 | TRP | 488 | 114.793 | 22.507 | 43.237 | 1.00 | 18.03 |
| | 4623 | CZ2 | TRP | 488 | 115.305 | 24.863 | 44.736 | 1.00 | 16.71 |
| 5 | 4624 | CZ3 | TRP | 488 | 115.654 | 23.499 | 42.765 | 1.00 | 15.24 |
| | 4625 | CH2 | TRP | 488 | 115.899 | 24.659 | 43.515 | 1.00 | 14.14 |
| | 4626 | H | TRP | 488 | 110.109 | 20.905 | 45.009 | 1.00 | 25.00 |
| | 4627 | HE1 | TRP | 488 | 113.699 | 24.482 | 47.075 | 1.00 | 25.00 |
| | 4628 | N | LYS | 489 | 111.136 | 18.399 | 43.138 | 1.00 | 21.51 |
| 10 | 4629 | CA | LYS | 489 | 111.162 | 17.175 | 42.345 | 1.00 | 17.89 |
| | 4630 | C | LYS | 489 | 110.604 | 17.476 | 40.961 | 1.00 | 19.66 |
| | 4631 | O | LYS | 489 | 111.091 | 16.947 | 39.960 | 1.00 | 22.89 |
| | 4632 | CB | LYS | 489 | 110.351 | 16.069 | 43.019 | 1.00 | 17.77 |
| | 4633 | CG | LYS | 489 | 110.922 | 15.624 | 44.344 | 1.00 | 15.98 |
| 15 | 4634 | CD | LYS | 489 | 110.074 | 14.540 | 44.972 | 1.00 | 22.31 |
| | 4635 | CE | LYS | 489 | 110.525 | 14.254 | 46.392 | 1.00 | 24.45 |
| | 4636 | NZ | LYS | 489 | 109.694 | 13.199 | 47.029 | 1.00 | 26.46 |
| | 4637 | H | LYS | 489 | 110.589 | 18.443 | 43.952 | 1.00 | 25.00 |
| | 4638 | 1HZ | LYS | 489 | 108.703 | 13.510 | 47.052 | 1.00 | 25.00 |
| 20 | 4639 | 2HZ | LYS | 489 | 109.772 | 12.320 | 46.482 | 1.00 | 25.00 |
| | 4640 | 3HZ | LYS | 489 | 110.028 | 13.037 | 47.997 | 1.00 | 25.00 |
| | 4641 | N | ASP | 490 | 109.590 | 18.338 | 40.906 | 1.00 | 20.77 |
| | 4642 | CA | ASP | 490 | 108.991 | 18.721 | 39.630 | 1.00 | 21.97 |
| | 4643 | C | ASP | 490 | 110.008 | 19.479 | 38.786 | 1.00 | 24.19 |
| 25 | 4644 | O | ASP | 490 | 110.098 | 19.264 | 37.575 | 1.00 | 21.17 |
| | 4645 | CB | ASP | 490 | 107.739 | 19.585 | 39.837 | 1.00 | 26.18 |
| | 4646 | CG | ASP | 490 | 106.561 | 18.799 | 40.395 | 1.00 | 29.44 |
| | 4647 | OD1 | ASSP | 490 | 106.524 | 17.562 | 40.236 | 1.00 | 35.64 |
| | 4648 | OD2 | ASP | 490 | 105.657 | 19.425 | 40.982 | 1.00 | 29.87 |
| 30 | 4649 | H | ASP | 490 | 109.245 | 18.731 | 41.736 | 1.00 | 25.00 |
| | 4650 | N | ILE | 491 | 110.776 | 20.362 | 39.419 | 1.00 | 20.68 |
| | 4651 | CA | ILE | 491 | 111.789 | 21.120 | 38.692 | 1.00 | 20.37 |
| | 4652 | C | ILE | 491 | 112.810 | 20.146 | 38.115 | 1.00 | 19.25 |
| | 4653 | O | ILE | 491 | 113.158 | 20.221 | 36.934 | 1.00 | 20.39 |
| 35 | 4654 | CB | ILE | 491 | 112.508 | 22.153 | 39.595 | 1.00 | 22.00 |
| | 4655 | CG1 | ILE | 491 | 111.540 | 23.278 | 39.975 | 1.00 | 21.39 |
| | 4656 | CG2 | ILE | 491 | 113.737 | 22.716 | 38.877 | 1.00 | 21.00 |
| | 4657 | CD1 | ILE | 491 | 112.159 | 24.376 | 40.803 | 1.00 | 22.99 |
| | 4658 | H | ILE | 491 | 110.657 | 20.508 | 40.379 | 1.00 | 25.00 |
| 40 | 4659 | N | ASN | 492 | 113.239 | 19.198 | 38.943 | 1.00 | 19.07 |
| | 4660 | CA | ASN | 492 | 114.216 | 18.196 | 38.529 | 1.00 | 18.67 |
| | 4661 | C | ASN | 492 | 113.700 | 17.404 | 37.332 | 1.00 | 20.34 |
| | 4662 | O | ASN | 492 | 114.446 | 17.133 | 36.393 | 1.00 | 20.40 |
| | 4663 | CB | ASN | 492 | 114.567 | 17.271 | 39.699 | 1.00 | 16.62 |
| 45 | 4664 | CG | ASN | 492 | 115.269 | 18.007 | 40.839 | 1.00 | 18.56 |
| | 4665 | OD1 | ASN | 492 | 115.924 | 19.035 | 40.625 | 1.00 | 15.51 |
| | 4666 | ND2 | ASN | 492 | 115.140 | 17.484 | 42.050 | 1.00 | 15.73 |
| | 4667 | H | ASN | 492 | 112.899 | 19.181 | 39.862 | 1.00 | 25.00 |
| | 4668 | 1HD2 | ASN | 492 | 115.583 | 17.939 | 42.793 | 1.00 | 25.00 |
| 50 | 4669 | 2HD2 | ASN | 492 | 114.613 | 16.661 | 42.164 | 1.00 | 25.00 |
| | 4670 | N | GLU | 493 | 112.412 | 17.073 | 37.341 | 1.00 | 21.12 |
| | 4671 | CA | GLU | 493 | 111.816 | 16.341 | 36.225 | 1.00 | 22.19 |

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|----|-------|------|-----|-----|---------|--------|--------|------|-------|
| | 4672 | C | GLU | 493 | 111.736 | 17.225 | 34.985 | 1.00 | 24.12 |
| | 4673 | O | GLU | 493 | 111.958 | 16.755 | 33.869 | 1.00 | 26.10 |
| | 4674 | CB | GLU | 493 | 110.416 | 15.850 | 36.578 | 1.00 | 19.71 |
| | 4675 | CG | GLU | 493 | 110.394 | 14.831 | 37.690 | 1.00 | 30.24 |
| 5 | 4676 | CD | GLU | 493 | 109.056 | 14.143 | 37.849 | 1.00 | 25.61 |
| | 4677 | OE1 | GLU | 493 | 108.111 | 14.460 | 37.100 | 1.00 | 36.10 |
| | 4678 | OE2 | GLU | 493 | 108.953 | 13.268 | 38.728 | 1.00 | 35.77 |
| | 4679 | H | GLU | 493 | 111.859 | 17.328 | 38.111 | 1.00 | 25.00 |
| | 4680 | N | GLY | 494 | 111.423 | 18.504 | 35.194 | 1.00 | 24.81 |
| 10 | 4681 | CA | GLY | 494 | 111.311 | 19.451 | 34.096 | 1.00 | 18.06 |
| | 4682 | C | GLY | 494 | 112.614 | 19.686 | 33.352 | 1.00 | 25.75 |
| | 4683 | O | GLY | 494 | 112.605 | 20.176 | 32.217 | 1.00 | 25.47 |
| | 4684 | H | GLY | 494 | 111.263 | 18.819 | 36.107 | 1.00 | 25.00 |
| | 46885 | N | LEU | 495 | 113.735 | 19.350 | 33.986 | 1.00 | 24.09 |
| 15 | 4686 | CA | LEU | 495 | 115.047 | 19.523 | 33.367 | 1.00 | 23.57 |
| | 4687 | C | LEU | 495 | 115.465 | 18.331 | 32.503 | 1.00 | 23.66 |
| | 4688 | O | LEU | 495 | 116.385 | 18.445 | 31.700 | 1.00 | 25.21 |
| | 4689 | CB | LEU | 495 | 116.111 | 19.781 | 34.439 | 1.00 | 21.29 |
| | 4690 | CG | LEU | 495 | 115.968 | 21.063 | 35.270 | 1.00 | 24.69 |
| 20 | 4691 | CD1 | LEU | 495 | 116.913 | 21.024 | 36.459 | 1.00 | 15.49 |
| | 4692 | CD2 | LEU | 495 | 116.230 | 22.287 | 34.409 | 1.00 | 21.41 |
| | 4693 | H | LEU | 495 | 113.681 | 18.985 | 34.893 | 1.00 | 25.00 |
| | 4694 | N | LEU | 496 | 114.781 | 17.200 | 32.651 | 1.00 | 22.59 |
| | 4695 | CA | LEU | 496 | 115.118 | 15.996 | 31.889 | 1.00 | 20.47 |
| 25 | 4696 | C | LEU | 496 | 114.749 | 16.049 | 30.409 | 1.00 | 24.46 |
| | 4697 | O | LEU | 496 | 113.692 | 16.556 | 30.033 | 1.00 | 22.73 |
| | 4698 | CB | LEU | 496 | 114.504 | 14.758 | 32.548 | 1.00 | 20.18 |
| | 4699 | CG | LEU | 496 | 115.016 | 14.454 | 33.959 | 1.00 | 23.38 |
| | 4700 | CD1 | LEU | 496 | 114.276 | 13.265 | 34.524 | 1.00 | 21.31 |
| 30 | 4701 | CD2 | LEU | 496 | 116.523 | 14.187 | 33.938 | 1.00 | 20.33 |
| | 4702 | H | LEU | 496 | 114.020 | 17.172 | 33.267 | 1.00 | 25.00 |
| | 4703 | N | ARG | 497 | 115.642 | 15.530 | 29.573 | 1.00 | 26.43 |
| | 4704 | CA | ARG | 497 | 115.443 | 15.501 | 28.128 | 1.00 | 31.12 |
| | 4705 | C | ARG | 497 | 114.347 | 14.498 | 27.766 | 1.00 | 32.68 |
| 35 | 4706 | O | ARG | 497 | 114.217 | 13.457 | 28.411 | 1.00 | 27.55 |
| | 4707 | CB | ARG | 497 | 116.757 | 15.124 | 27.431 | 1.00 | 30.06 |
| | 4708 | CG | ARG | 497 | 117.863 | 16.155 | 27.626 | 1.00 | 38.94 |
| | 4709 | CD | ARG | 497 | 119.217 | 15.505 | 27.851 | 1.00 | 37.77 |
| | 4710 | NE | ARG | 497 | 120.087 | 15.584 | 26.683 | 1.00 | 50.61 |
| 40 | 4711 | CZ | ARG | 497 | 121.282 | 16.173 | 26.676 | 1.00 | 51.72 |
| | 4712 | NH1 | ARG | 497 | 121.754 | 16.744 | 27.777 | 1.00 | 46.52 |
| | 4713 | NH2 | ARG | 497 | 122.023 | 16.166 | 25.575 | 1.00 | 51.65 |
| | 4714 | H | ARG | 497 | 116.457 | 15.140 | 29.946 | 1.00 | 25.00 |
| | 4715 | HE | ARG | 497 | 119.773 | 15.180 | 25.847 | 1.00 | 25.00 |
| 45 | 4716 | 1HH1 | ARG | 497 | 121.213 | 16.733 | 28.615 | 1.00 | 25.00 |
| | 4717 | 2HH1 | ARG | 497 | 122.653 | 17.183 | 27.766 | 1.00 | 25.00 |
| | 4718 | 1HH2 | ARG | 497 | 121.685 | 15.718 | 24.748 | 1.00 | 25.00 |
| | 4719 | 2HH2 | ARG | 497 | 122.920 | 16.608 | 25.576 | 1.00 | 25.00 |
| | 4720 | N | PRO | 498 | 113.542 | 14.798 | 26.731 | 1.00 | 34.46 |
| 50 | 4721 | CA | PRO | 498 | 113.595 | 16.005 | 25.897 | 1.00 | 31.05 |
| | 4722 | C | PRO | 498 | 112.886 | 17.179 | 26.568 | 1.00 | 32.44 |
| | 4723 | O | PRO | 498 | 111.757 | 17.040 | 27.043 | 1.00 | 32.35 |

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|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 4724 | CB | PRO | 498 | 112.831 | 15.587 | 24.635 | 1.00 | 30.63 |
| | 4725 | CG | PRO | 498 | 112.768 | 14.079 | 24.707 | 1.00 | 38.95 |
| | 4726 | CD | PRO | 498 | 112.593 | 13.830 | 26.162 | 1.00 | 34.35 |
| | 4727 | N | THR | 499 | 113.544 | 18.332 | 26.612 | 1.00 | 33.10 |
| 5 | 4728 | CA | THR | 499 | 112.940 | 19.513 | 27.218 | 1.00 | 30.18 |
| | 4729 | C | THR | 499 | 112.075 | 20.223 | 26.170 | 1.00 | 31.00 |
| | 4730 | O | THR | 499 | 112.369 | 20.172 | 24.974 | 1.00 | 33.56 |
| | 4731 | CB | THR | 499 | 114.016 | 20.474 | 27.795 | 1.00 | 25.39 |
| | 4732 | OG1 | THR | 499 | 115.004 | 20.752 | 26.798 | 1.00 | 24.84 |
| 10 | 4733 | CG2 | THR | 499 | 114.703 | 19.843 | 28.996 | 1.00 | 22.98 |
| | 4734 | H | THR | 499 | 114.435 | 18.421 | 26.223 | 1.00 | 25.00 |
| | 4735 | HG1 | THR | 499 | 115.646 | 21.357 | 27.117 | 1.00 | 25.00 |
| | 4736 | N | PRO | 500 | 110.963 | 20.844 | 26.600 | 1.00 | 31.06 |
| | 4737 | CA | PRO | 500 | 110.053 | 21.558 | 25.692 | 1.00 | 32.31 |
| 15 | 4738 | C | PRO | 500 | 110.705 | 22.740 | 24.967 | 1.00 | 34.94 |
| | 4739 | O | PRO | 500 | 110.328 | 23.075 | 23.843 | 1.00 | 39.31 |
| | 4740 | CB | PRO | 500 | 108.916 | 21.994 | 26.620 | 1.00 | 29.71 |
| | 4741 | CG | PRO | 500 | 109.576 | 22.086 | 27.968 | 1.00 | 28.06 |
| | 4742 | CD | PRO | 500 | 110.460 | 20.876 | 27.984 | 1.00 | 23.70 |
| 20 | 4743 | N | VAL | 501 | 111.642 | 23.398 | 25.641 | 1.00 | 32.94 |
| | 4744 | CA | VAL | 501 | 112.390 | 24.523 | 25.078 | 1.00 | 33.22 |
| | 4745 | C | VAL | 501 | 113.858 | 24.257 | 25.421 | 1.00 | 33.52 |
| | 4746 | O | VAL | 501 | 114.154 | 23.347 | 26.204 | 1.00 | 33.00 |
| | 4747 | CB | VAL | 501 | 111.959 | 25.887 | 25.686 | 1.00 | 29.14 |
| 25 | 4748 | CG1 | VAL | 501 | 110.515 | 26.198 | 25.330 | 1.00 | 26.33 |
| | 4749 | CG2 | VAL | 501 | 112.153 | 25.887 | 27.195 | 1.00 | 24.60 |
| | 4750 | H | VAL | 501 | 111.875 | 23.112 | 26.546 | 1.00 | 25.00 |
| | 4751 | N | SER | 502 | 114.775 | 25.026 | 24.844 | 1.00 | 30.56 |
| | 4752 | CA | SER | 502 | 116.194 | 24.832 | 25.128 | 1.00 | 33.20 |
| 30 | 4753 | C | SER | 502 | 116.485 | 25.025 | 26.611 | 1.00 | 32.05 |
| | 4754 | O | SER | 502 | 115.869 | 25.869 | 27.265 | 1.00 | 34.57 |
| | 4755 | CB | SER | 502 | 117.039 | 25.807 | 24.316 | 1.00 | 35.54 |
| | 4756 | OG | SER | 502 | 116.837 | 25.601 | 22.934 | 1.00 | 56.52 |
| | 4757 | H | SER | 502 | 114.502 | 25.729 | 24.224 | 1.00 | 25.00 |
| 35 | 4758 | HG | SER | 502 | 117.098 | 24.709 | 22.686 | 1.00 | 25.00 |
| | 4759 | N | THR | 503 | 117.443 | 24.260 | 27.126 | 1.00 | 29.15 |
| | 4760 | CA | THR | 503 | 117.836 | 24.333 | 28.530 | 1.00 | 33.23 |
| | 4761 | C | THR | 503 | 118.166 | 25.771 | 28.927 | 1.00 | 31.90 |
| | 4762 | O | THR | 503 | 117.977 | 26.177 | 30.078 | 1.00 | 32.13 |
| 40 | 4763 | CB | THR | 503 | 119.058 | 23.443 | 28.797 | 1.00 | 38.70 |
| | 4764 | OG1 | THR | 503 | 118.767 | 22.110 | 28.366 | 1.00 | 51.69 |
| | 4765 | CG2 | THR | 503 | 119.395 | 23.420 | 30.278 | 1.00 | 40.66 |
| | 4766 | H | THR | 503 | 117.884 | 23.611 | 26.547 | 1.00 | 25.00 |
| | 4767 | HG1 | THR | 503 | 118.560 | 22.075 | 27.436 | 1.00 | 25.00 |
| 45 | 4768 | N | GLU | 504 | 118.637 | 26.542 | 27.956 | 1.00 | 27.88 |
| | 4769 | CA | GLU | 504 | 118.982 | 27.935 | 28.184 | 1.00 | 31.30 |
| | 4770 | C | GLU | 504 | 117.801 | 28.706 | 28.789 | 1.00 | 31.46 |
| | 4771 | O | GLU | 504 | 117.987 | 29.643 | 29.568 | 1.00 | 29.72 |
| | 4772 | CB | GLU | 504 | 119.396 | 28.578 | 26.863 | 1.00 | 32.18 |
| 50 | 4773 | CG | GLU | 504 | 119.754 | 30.042 | 26.997 | 1.00 | 44.47 |
| | 4774 | CD | GLU | 504 | 120.045 | 30.714 | 25.672 | 1.00 | 47.35 |
| | 4775 | OE1 | GLU | 504 | 119.634 | 30.183 | 24.618 | 1.00 | 49.18 |

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|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 4776 | OE2 | GLU | 504 | 120.683 | 31.788 | 25.691 | 1.00 | 48.31 |
| | 4777 | H | GLU | 504 | 118.771 | 26.169 | 27.067 | 1.00 | 25.00 |
| | 4778 | N | PHE | 505 | 116.588 | 28.274 | 28.464 | 1.00 | 27.10 |
| | 4779 | CA | PHE | 505 | 115.390 | 28.936 | 28.957 | 1.00 | 23.02 |
| 5 | 4780 | C | PHE | 505 | 114.809 | 28.314 | 30.218 | 1.00 | 24.14 |
| | 4781 | O | PHE | 505 | 113.888 | 28.869 | 30.818 | 1.00 | 22.77 |
| | 4782 | CB | PHE | 505 | 114.356 | 29.036 | 27.835 | 1.00 | 28.22 |
| | 4783 | CG | PHE | 505 | 114.888 | 29.711 | 26.602 | 1.00 | 28.58 |
| | 4784 | CD1 | PHE | 505 | 115.307 | 31.039 | 26.651 | 1.00 | 28.23 |
| 10 | 4785 | CD2 | PHE | 505 | 115.048 | 29.001 | 25.417 | 1.00 | 28.81 |
| | 4786 | CE1 | PHE | 505 | 115.884 | 31.646 | 25.539 | 1.00 | 25.11 |
| | 4787 | CE2 | PHE | 505 | 115.623 | 29.597 | 24.300 | 1.00 | 28.43 |
| | 4788 | CZ | PHE | 505 | 116.043 | 30.922 | 24.362 | 1.00 | 29.72 |
| | 4789 | H | PHE | 505 | 116.489 | 27.504 | 27.881 | 1.00 | 25.00 |
| 15 | 4790 | N | LEU | 506 | 115.367 | 27.182 | 30.641 | 1.00 | 21.53 |
| | 4791 | CA | LEU | 506 | 114.915 | 26.516 | 31.862 | 1.00 | 20.00 |
| | 4792 | C | LEU | 506 | 115.763 | 26.980 | 33.054 | 1.00 | 20.28 |
| | 4793 | O | LEU | 506 | 115.270 | 27.120 | 34.176 | 1.00 | 21.38 |
| | 4794 | CB | LEU | 506 | 115.033 | 24.995 | 31.732 | 1.00 | 17.84 |
| 20 | 4795 | CG | LEU | 506 | 114.265 | 24.277 | 30.621 | 1.00 | 23.70 |
| | 4796 | CD1 | LEU | 506 | 114.409 | 22.781 | 30.832 | 1.00 | 19.27 |
| | 4797 | CD2 | LEU | 506 | 112.797 | 24.671 | 30.645 | 1.00 | 20.22 |
| | 4798 | H | LEU | 506 | 116.092 | 26.791 | 30.120 | 1.00 | 25.00 |
| | 4799 | N | THR | 507 | 117.040 | 27.237 | 32.796 | 1.00 | 24.00 |
| 25 | 4800 | CA | THR | 507 | 117.968 | 27.666 | 33.837 | 1.00 | 21.87 |
| | 4801 | C | THR | 507 | 117.508 | 28.894 | 34.634 | 1.00 | 21.92 |
| | 4802 | O | THR | 507 | 117.636 | 28.913 | 35.858 | 1.00 | 25.77 |
| | 4803 | CB | THR | 507 | 119.382 | 27.870 | 33.260 | 1.00 | 22.57 |
| | 4804 | OG1 | THR | 507 | 119.728 | 26.728 | 32.465 | 1.00 | 23.76 |
| 30 | 4805 | CG2 | THR | 507 | 120.400 | 28.014 | 34.381 | 1.00 | 20.42 |
| | 4806 | H | THR | 507 | 117.372 | 27.127 | 31.883 | 1.00 | 25.00 |
| | 4807 | HG1 | THR | 507 | 119.106 | 26.624 | 31.739 | 1.00 | 25.00 |
| | 4808 | N | PRO | 508 | 116.960 | 29.928 | 33.963 | 1.00 | 17.26 |
| | 4809 | CA | PRO | 508 | 116.503 | 31.114 | 34.698 | 1.00 | 18.03 |
| 35 | 4810 | C | PRO | 508 | 115.423 | 30.774 | 35.735 | 1.00 | 19.69 |
| | 4811 | O | PRO | 508 | 115.417 | 31.309 | 36.847 | 1.00 | 22.29 |
| | 4812 | CB | PRO | 508 | 115.943 | 31.999 | 33.583 | 1.00 | 18.28 |
| | 4813 | CG | PRO | 508 | 116.841 | 31.690 | 32.444 | 1.00 | 16.25 |
| | 4814 | CD | PRO | 508 | 116.909 | 30.177 | 32.510 | 1.00 | 14.75 |
| 40 | 4815 | N | ILE | 509 | 114.528 | 29.864 | 35.362 | 1.00 | 21.35 |
| | 4816 | CA | ILE | 509 | 113.435 | 29.420 | 36.230 | 1.00 | 22.73 |
| | 4817 | C | ILE | 509 | 114.024 | 28.653 | 37.412 | 1.00 | 19.96 |
| | 4818 | O | ILE | 509 | 113.627 | 28.854 | 38.561 | 1.00 | 22.40 |
| | 4819 | CB | ILE | 509 | 112.450 | 28.523 | 35.441 | 1.00 | 18.26 |
| 45 | 4820 | CG1 | ILE | 509 | 111.867 | 29.317 | 34.267 | 1.00 | 20.40 |
| | 4821 | CG2 | ILE | 509 | 111.360 | 27.998 | 36.351 | 1.00 | 12.67 |
| | 4822 | CD1 | ILE | 509 | 111.082 | 28.486 | 33.280 | 1.00 | 22.89 |
| | 4823 | H | ILE | 509 | 114.597 | 29.468 | 34.470 | 1.00 | 25.00 |
| | 4824 | N | LEU | 510 | 114.989 | 27.788 | 37.114 | 1.00 | 21.34 |
| 50 | 4825 | CA | LEU | 510 | 115.684 | 27.003 | 38.130 | 1.00 | 19.45 |
| | 4826 | C | LEU | 510 | 116.420 | 27.956 | 39.075 | 1.00 | 18.03 |
| | 4827 | O | LEU | 510 | 116.372 | 27.799 | 40.300 | 1.00 | 23.54 |

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|----|------|------|-----|------|---------|---------|--------|------|-------|
| | 4828 | CB | LEU | 510 | 116.693 | 26.064 | 37.454 | 1.00 | 18.99 |
| | 4829 | CG | LEU | 510 | 117.747 | 25.351 | 38.309 | 1.00 | 17.88 |
| | 4830 | CD1 | LEU | 510 | 117.092 | 24.447 | 39.347 | 1.00 | 13.70 |
| | 4831 | CD2 | LEU | 510 | 118.660 | 24.548 | 37.401 | 1.00 | 12.82 |
| 5 | 4832 | H | LEU | 510 | 115.234 | 27.670 | 36.174 | 1.00 | 25.00 |
| | 4833 | N | ASN | 511 | 117.070 | 28.966 | 38.502 | 1.00 | 16.84 |
| | 4834 | CA | ASN | 511 | 117.816 | 29.940 | 39.293 | 1.00 | 18.52 |
| | 4835 | C | ASN | 511 | 116.918 | 30.774 | 40.185 | 1.00 | 19.49 |
| | 4836 | O | ASN | 511 | 117.299 | 31.111 | 41.307 | 1.00 | 21.10 |
| 10 | 4837 | CB | ASN | 511 | 118.704 | 30.806 | 38.400 | 1.00 | 14.99 |
| | 4838 | CG | ASN | 511 | 119.926 | 30.046 | 37.903 | 1.00 | 19.61 |
| | 4839 | OD1 | ASN | 511 | 120.276 | 29.004 | 38.456 | 1.00 | 22.94 |
| | 4840 | ND2 | ASN | 511 | 120.562 | 30.543 | 36.849 | 1.00 | 17.54 |
| | 4841 | H | ASN | 511 | 117.040 | 29.059 | 37.540 | 1.00 | 25.00 |
| 15 | 4842 | 1HD2 | ASN | 511 | 121.341 | 30.052 | 36.532 | 1.00 | 25.00 |
| | 4843 | 2HD2 | ASN | 511 | 120.230 | 31.364 | 36.438 | 1.00 | 25.00 |
| | 4844 | N | LEU | 512 | 115.705 | 31.061 | 39.719 | 1.00 | 18.46 |
| | 4845 | CA | LEU | 512 | 114.751 | 31.814 | 40.527 | 1.00 | 15.00 |
| | 4846 | C | LEU | 512 | 114.415 | 31.007 | 41.778 | 1.00 | 16.15 |
| 20 | 4847 | O | LEU | 512 | 114.304 | 31.561 | 42.872 | 1.00 | 24.00 |
| | 4848 | CB | LEU | 512 | 113.484 | 32.114 | 39.727 | 1.00 | 17.19 |
| | 4849 | CG | LEU | 5112 | 113.569 | 33.341 | 38.818 | 1.00 | 16.79 |
| | 4850 | CD1 | LEU | 512 | 112.331 | 33.430 | 37.943 | 1.00 | 22.39 |
| | 4851 | CD2 | LEU | 512 | 113.702 | 34.591 | 39.672 | 1.00 | 14.37 |
| 25 | 4852 | H | LEU | 512 | 115.450 | 30.773 | 38.817 | 1.00 | 25.00 |
| | 4853 | N | ALA | 513 | 114.279 | 29.692 | 41.624 | 1.00 | 19.31 |
| | 4854 | CA | ALA | 513 | 113.979 | 28.814 | 42.760 | 1.00 | 18.01 |
| | 4855 | C | ALA | 513 | 115.178 | 28.789 | 43.710 | 1.00 | 18.19 |
| | 4856 | O | ALA | 513 | 115.017 | 28.802 | 44.933 | 1.00 | 16.94 |
| 30 | 4857 | CB | ALA | 513 | 113.654 | 27.403 | 42.274 | 1.00 | 12.64 |
| | 4858 | H | ALA | 513 | 114.362 | 29.302 | 40.726 | 1.00 | 25.00 |
| | 4859 | N | ARG | 514 | 116.381 | 28.767 | 43.140 | 1.00 | 19.70 |
| | 4860 | CA | ARG | 514 | 117.609 | 28.763 | 43.934 | 1.00 | 18.80 |
| | 4861 | C | ARG | 514 | 117.696 | 30.031 | 44.784 | 1.00 | 17.46 |
| 35 | 4862 | O | ARG | 514 | 118.041 | 29.978 | 45.967 | 1.00 | 21.48 |
| | 4863 | CB | ARG | 514 | 118.832 | 28.638 | 43.024 | 1.00 | 13.68 |
| | 4864 | CG | ARG | 514 | 118.981 | 27.255 | 42.404 | 1.00 | 14.32 |
| | 4865 | CD | ARG | 514 | 120.084 | 27.218 | 41.354 | 1.00 | 17.33 |
| | 4866 | NE | ARG | 514 | 120.490 | 25.848 | 41.066 | 1.00 | 16.97 |
| 40 | 4867 | CZ | ARG | 514 | 121.107 | 25.453 | 39.958 | 1.00 | 19.03 |
| | 4868 | NH1 | ARG | 514 | 121.398 | 26.320 | 38.998 | 1.00 | 15.08 |
| | 4869 | NH2 | ARG | 514 | 121.450 | 24.180 | 39.821 | 1.00 | 15.36 |
| | 4870 | H | ARG | 514 | 116.440 | 28.744 | 42.160 | 1.00 | 25.00 |
| | 4871 | HE | ARG | 514 | 120.282 | 25.180 | 41.738 | 1.00 | 25.00 |
| 45 | 4872 | 1HH1 | ARG | 514 | 121.159 | 27.283 | 39.100 | 1.00 | 25.00 |
| | 4873 | 2HH1 | ARG | 514 | 121.862 | 26.006 | 38.170 | 1.00 | 25.00 |
| | 4874 | 1HH2 | ARG | 514 | 121.245 | 23.5244 | 40.547 | 1.00 | 25.00 |
| | 4875 | 2HH2 | ARG | 514 | 121.913 | 23.875 | 38.988 | 1.00 | 25.00 |
| | 4876 | N | ILE | 515 | 117.330 | 31.164 | 44.196 | 1.00 | 20.52 |
| 50 | 4877 | CA | ILE | 515 | 117.352 | 32.438 | 44.911 | 1.00 | 22.89 |
| | 4878 | C | ILE | 515 | 116.489 | 32.357 | 46.169 | 1.00 | 25.55 |
| | 4879 | O | ILE | 515 | 116.851 | 32.914 | 47.206 | 1.00 | 28.26 |

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|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 4880 | CB | ILE | 515 | 116.863 | 33.591 | 44.018 | 1.00 | 18.86 |
| | 4881 | CG1 | ILE | 515 | 117.857 | 33.824 | 42.883 | 1.00 | 18.35 |
| | 4882 | CG2 | ILE | 515 | 116.695 | 34.855 | 44.832 | 1.00 | 23.30 |
| | 4883 | CD1 | ILE | 515 | 117.408 | 34.863 | 41.885 | 1.00 | 19.17 |
| 5 | 4884 | H | ILE | 515 | 117.045 | 31.141 | 43.257 | 1.00 | 25.00 |
| | 4885 | N | VAL | 516 | 115.372 | 31.637 | 46.082 | 1.00 | 27.24 |
| | 4886 | CA | VAL | 516 | 114.467 | 31.463 | 47.220 | 1.00 | 26.85 |
| | 4887 | C | VAL | 516 | 115.229 | 30.838 | 48.378 | 1.00 | 30.63 |
| | 4888 | O | VAL | 516 | 115.219 | 31.354 | 49.496 | 1.00 | 28.87 |
| 10 | 4889 | CB | VAL | 516 | 113.280 | 30.512 | 46.881 | 1.00 | 28.84 |
| | 4890 | CG1 | VAL | 516 | 112.433 | 30.248 | 48.122 | 1.00 | 23.42 |
| | 4891 | CG2 | VAL | 516 | 112.423 | 31.096 | 45.776 | 1.00 | 22.08 |
| | 4892 | H | VAL | 516 | 115.144 | 31.219 | 45.225 | 1.00 | 25.00 |
| | 4893 | N | GLU | 517 | 115.910 | 29.736 | 48.085 | 1.00 | 35.61 |
| 15 | 4894 | CA | GLU | 517 | 116.680 | 28.997 | 49.081 | 1.00 | 41.24 |
| | 4895 | C | GLU | 517 | 117.696 | 29.890 | 49.796 | 1.00 | 42.08 |
| | 4896 | O | GLU | 517 | 117.872 | 29.789 | 51.009 | 1.00 | 46.37 |
| | 4897 | CB | GLU | 517 | 117.385 | 27.802 | 48.424 | 1.00 | 41.58 |
| | 4898 | CG | GLU | 517 | 116.496 | 26.950 | 47.503 | 1.00 | 52.96 |
| 20 | 4899 | CD | GLU | 517 | 115.344 | 26.242 | 48.223 | 1.00 | 59.58 |
| | 4900 | OE1 | GLU | 517 | 115.593 | 25.557 | 49.236 | 1.00 | 60.41 |
| | 4901 | OE2 | GLU | 517 | 114.187 | 26.352 | 47.762 | 1.00 | 63.04 |
| | 4902 | H | GLU | 517 | 115.899 | 29.407 | 47.161 | 1.00 | 25.00 |
| | 4903 | N | VAL | 518 | 118.314 | 30.799 | 49.050 | 1.00 | 40.18 |
| 25 | 4904 | CA | VAL | 518 | 119.310 | 31.714 | 49.600 | 1.00 | 42.32 |
| | 4905 | C | VAL | 518 | 118.704 | 32.885 | 50.386 | 1.00 | 47.45 |
| | 4906 | O | VAL | 518 | 119.269 | 33.326 | 51.389 | 1.00 | 48.49 |
| | 4907 | CB | VAL | 518 | 120.219 | 32.251 | 48.474 | 1.00 | 41.14 |
| | 4908 | CG1 | VAL | 518 | 121.133 | 33.350 | 48.986 | 1.00 | 39.83 |
| 30 | 4909 | CG2 | VAL | 518 | 121.034 | 31.108 | 47.896 | 1.00 | 45.30 |
| | 4910 | H | VAL | 518 | 118.097 | 30.844 | 48.095 | 1.00 | 25.00 |
| | 4911 | N | THR | 519 | 117.563 | 33.387 | 49.923 | 1.00 | 45.49 |
| | 4912 | CA | THR | 519 | 116.899 | 34.505 | 50.577 | 1.00 | 44.49 |
| | 4913 | C | THR | 519 | 116.183 | 34.117 | 51.884 | 1.00 | 44.03 |
| 35 | 4914 | O | THR | 519 | 115.983 | 34.964 | 52.754 | 1.00 | 41.48 |
| | 4915 | CB | THR | 519 | 115.868 | 35.165 | 49.622 | 1.00 | 45.40 |
| | 4916 | OG1 | THR | 519 | 116.518 | 35.516 | 48.394 | 1.00 | 47.45 |
| | 4917 | CG2 | THR | 519 | 115.283 | 36.424 | 50.240 | 1.00 | 50.81 |
| | 4918 | H | THR | 519 | 117.161 | 32.996 | 49.123 | 1.00 | 25.00 |
| 40 | 4919 | HG1 | THR | 519 | 116.872 | 34.719 | 47.980 | 1.00 | 25.00 |
| | 4920 | N | TYR | 520 | 115.827 | 32.843 | 52.034 | 1.00 | 49.74 |
| | 4921 | CA | TYR | 520 | 115.130 | 32.385 | 53.240 | 1.00 | 54.71 |
| | 4922 | C | TYR | 520 | 115.783 | 31.213 | 53.984 | 1.00 | 60.58 |
| | 4923 | O | TYR | 520 | 115.129 | 30.191 | 54.209 | 1.00 | 65.16 |
| 45 | 4924 | CB | TYR | 520 | 113.686 | 31.988 | 52.905 | 1.00 | 52.58 |
| | 4925 | CG | TYR | 520 | 112.886 | 33.018 | 52.142 | 1.00 | 53.27 |
| | 4926 | CD1 | TYR | 520 | 112.885 | 33.027 | 50.748 | 1.00 | 54.77 |
| | 4927 | CD2 | TYR | 520 | 112.105 | 33.962 | 52.809 | 1.00 | 50.10 |
| | 4928 | CE1 | TYR | 520 | 112.127 | 33.946 | 50.032 | 1.00 | 57.50 |
| 50 | 4929 | CE2 | TYR | 520 | 111.340 | 34.889 | 52.102 | 1.00 | 54.19 |
| | 4930 | CZ | TYR | 520 | 111.357 | 34.873 | 50.713 | 1.00 | 56.86 |
| | 4931 | OH | TYR | 520 | 110.604 | 35.777 | 49.999 | 1.00 | 58.70 |

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|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 4932 | H | TYR | 520 | 116.029 | 32.189 | 51.330 | 1.00 | 25.00 |
| | 4933 | HH | TYR | 520 | 110.726 | 35.626 | 49.057 | 1.00 | 25.00 |
| | 4934 | N | ILE | 521 | 117.056 | 31.340 | 54.350 | 1.00 | 67.35 |
| | 4935 | CA | ILE | 521 | 117.729 | 30.269 | 55.091 | 1.00 | 74.89 |
| 5 | 4936 | C | ILE | 521 | 117.425 | 30.428 | 56.583 | 1.00 | 75.44 |
| | 4937 | O | ILE | 521 | 117.194 | 29.397 | 57.255 | 1.00 | 76.20 |
| | 4938 | CB | ILE | 521 | 119.276 | 30.258 | 54.856 | 1.00 | 75.70 |
| | 4939 | CG1 | ILE | 521 | 119.586 | 29.919 | 53.394 | 1.00 | 76.18 |
| | 4940 | CG2 | ILE | 521 | 119.953 | 29.222 | 55.766 | 1.00 | 77.50 |
| 10 | 4941 | CD1 | ILE | 521 | 121.064 | 29.755 | 53.080 | 1.00 | 71.61 |
| | 4942 | H | ILE | 521 | 117.546 | 32.156 | 54.145 | 1.00 | 25.00 |
| | 4943 | N | VAL | 533 | 120.428 | 39.967 | 55.248 | 1.00 | 55.02 |
| | 4944 | CA | VAL | 533 | 120.478 | 38.584 | 54.683 | 1.00 | 57.02 |
| | 4945 | C | VAL | 533 | 121.277 | 38.505 | 53.373 | 1.00 | 55.80 |
| 15 | 4946 | O | VAL | 533 | 122.075 | 37.588 | 53.181 | 1.00 | 56.73 |
| | 4947 | CB | VAL | 533 | 119.048 | 37.995 | 54.485 | 1.00 | 56.30 |
| | 4948 | CG1 | VAL | 533 | 118.225 | 38.868 | 53.539 | 1.00 | 56.90 |
| | 4949 | CG2 | VAL | 533 | 119.125 | 36.552 | 53.986 | 1.00 | 50.74 |
| | 4950 | 1H | VAL | 533 | 119.970 | 40.608 | 54.578 | 1.00 | 25.00 |
| 20 | 4951 | 2H | VAL | 533 | 119.880 | 39.938 | 56.132 | 1.00 | 25.00 |
| | 4952 | 3H | VAL | 533 | 121.396 | 40.274 | 55.462 | 1.00 | 25.00 |
| | 4953 | N | LEU | 534 | 121.095 | 39.483 | 52.491 | 1.00 | 49.61 |
| | 4954 | CA | LEU | 534 | 121.812 | 39.490 | 51.218 | 1.00 | 48.50 |
| | 4955 | C | LEU | 534 | 123.194 | 40.138 | 51.300 | 1.00 | 47.52 |
| 25 | 4956 | O | LEU | 534 | 124.075 | 39.830 | 50.496 | 1.00 | 44.98 |
| | 4957 | CB | LEU | 534 | 120.983 | 40.190 | 50.137 | 1.00 | 48.86 |
| | 4958 | CG | LEU | 534 | 119.659 | 39.533 | 49.744 | 1.00 | 50.00 |
| | 4959 | CD1 | LEU | 534 | 119.054 | 40.290 | 48.567 | 1.00 | 46.00 |
| | 4960 | CD2 | LEU | 534 | 119.886 | 38.066 | 49.384 | 1.00 | 42.36 |
| 30 | 4961 | H | LEU | 534 | 120.456 | 40.200 | 52.652 | 1.00 | 25.00 |
| | 4962 | N | LYS | 535 | 123.382 | 40.993 | 52.303 | 1.00 | 45.93 |
| | 4963 | CA | LYS | 535 | 124.633 | 41.722 | 52.510 | 1.00 | 45.11 |
| | 4964 | C | LYS | 535 | 125.921 | 40.923 | 52.284 | 1.00 | 43.08 |
| | 4965 | O | LYS | 535 | 126.729 | 41.288 | 51.428 | 1.00 | 42.36 |
| 35 | 4966 | CB | LYS | 535 | 124.651 | 42.385 | 53.895 | 1.00 | 46.19 |
| | 4967 | CG | LYS | 535 | 125.855 | 43.288 | 54.130 | 1.00 | 54.44 |
| | 4968 | CD | LYS | 535 | 125.868 | 43.868 | 55.536 | 1.00 | 57.76 |
| | 4969 | CE | LYS | 535 | 127.075 | 44.774 | 55.747 | 1.00 | 61.61 |
| | 4970 | NZ | LYS | 535 | 127.099 | 45.378 | 57.111 | 1.00 | 62.66 |
| 40 | 4971 | H | LYS | 535 | 122.651 | 41.156 | 52.915 | 1.00 | 25.00 |
| | 4972 | 1HZ | LYS | 535 | 127.134 | 44.621 | 57.824 | 1.00 | 25.00 |
| | 4973 | 2HZ | LYS | 535 | 127.936 | 45.986 | 57.207 | 1.00 | 25.00 |
| | 4974 | 3HZ | LYS | 535 | 126.239 | 45.946 | 57.252 | 1.00 | 25.00 |
| | 4975 | N | PRO | 536 | 126.115 | 39.809 | 53.019 | 1.00 | 39.15 |
| 45 | 4976 | CA | PRO | 536 | 127.337 | 39.020 | 52.829 | 1.00 | 37.51 |
| | 4977 | C | PRO | 536 | 127.564 | 38.579 | 51.386 | 1.00 | 33.92 |
| | 4978 | O | PRO | 536 | 128.684 | 38.644 | 50.877 | 1.00 | 33.28 |
| | 4979 | CB | PRO | 536 | 127.128 | 37.827 | 53.770 | 1.00 | 38.16 |
| | 4980 | CG | PRO | 536 | 125.638 | 37.724 | 53.893 | 1.00 | 42.17 |
| 50 | 4981 | CD | PRO | 536 | 125.233 | 39.164 | 54.008 | 1.00 | 38.53 |
| | 4982 | N | HIS | 537 | 126.488 | 38.181 | 50.714 | 1.00 | 33.98 |
| | 4983 | CA | HIS | 537 | 126.575 | 37.730 | 49.327 | 1.00 | 34.56 |

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|----|------|------|-----|-----|---------|--------|--------|------|-------|
| | 4984 | C | HIS | 537 | 126.929 | 38.877 | 48.390 | 1.00 | 34.75 |
| | 4985 | O | HIS | 537 | 127.742 | 38.714 | 47.479 | 1.00 | 29.05 |
| | 4986 | CB | HIS | 537 | 125.264 | 37.071 | 48.900 | 1.00 | 34.41 |
| | 4987 | CG | HIS | 537 | 124.917 | 35.855 | 49.703 | 1.00 | 41.27 |
| 5 | 4988 | ND1 | HIS | 537 | 123.749 | 35.746 | 50.426 | 1.00 | 43.98 |
| | 4989 | CD2 | HIS | 537 | 125.601 | 34.705 | 49.917 | 1.00 | 37.03 |
| | 4990 | CE1 | HIS | 537 | 123.726 | 34.584 | 51.053 | 1.00 | 40.28 |
| | 4991 | NE2 | HIS | 537 | 124.838 | 33.933 | 50.760 | 1.00 | 39.05 |
| | 4992 | H | HIS | 537 | 125.618 | 38.225 | 51.154 | 1.00 | 25.00 |
| 10 | 4993 | HD1 | HIS | 537 | 123.030 | 36.418 | 50.483 | 1.00 | 25.00 |
| | 4994 | HE2 | HIS | 537 | 125.072 | 33.038 | 51.088 | 1.00 | 25.00 |
| | 4995 | N | ILE | 538 | 126.333 | 40.040 | 48.634 | 1.00 | 34.95 |
| | 4996 | CA | ILE | 538 | 126.596 | 41.225 | 47.829 | 1.00 | 35.08 |
| | 4997 | C | ILE | 538 | 128.063 | 41.612 | 47.969 | 1.00 | 36.46 |
| 15 | 4998 | O | ILE | 538 | 128.703 | 41.999 | 46.990 | 1.00 | 38.58 |
| | 4999 | CB | ILE | 538 | 125.701 | 42.406 | 48.263 | 1.00 | 35.99 |
| | 5000 | CG1 | ILE | 538 | 124.230 | 42.072 | 47.983 | 1.00 | 37.36 |
| | 5001 | CG2 | ILE | 538 | 126.124 | 43.681 | 47.542 | 1.00 | 34.76 |
| | 5002 | CD1 | ILE | 538 | 123.248 | 43.112 | 48.460 | 1.00 | 36.39 |
| 20 | 5003 | H | ILE | 538 | 125.708 | 40.113 | 49.385 | 1.00 | 25.00 |
| | 5004 | N | ILE | 539 | 128.588 | 41.491 | 49.185 | 1.00 | 34.70 |
| | 5005 | CA | ILE | 539 | 129.979 | 41.807 | 49.473 | 1.00 | 33.68 |
| | 5006 | C | ILE | 539 | 130.912 | 40.828 | 48.769 | 1.00 | 34.74 |
| | 5007 | O | ILE | 539 | 131.868 | 41.239 | 48.093 | 1.00 | 30.49 |
| 25 | 5008 | CB | ILE | 539 | 130.253 | 41.761 | 51.004 | 1.00 | 35.37 |
| | 5009 | CG1 | ILE | 539 | 129.559 | 42.939 | 51.686 | 1.00 | 33.35 |
| | 5010 | CG2 | ILE | 539 | 131.749 | 41.790 | 51.285 | 1.00 | 32.80 |
| | 5011 | CD1 | ILE | 539 | 129.684 | 42.933 | 53.189 | 1.00 | 34.58 |
| | 5012 | H | ILE | 539 | 127.999 | 41.207 | 49.913 | 1.00 | 25.00 |
| 30 | 5013 | N | ASN | 540 | 130.603 | 39.538 | 48.864 | 1.00 | 33.09 |
| | 5014 | CA | ASN | 540 | 131.440 | 38.505 | 48.263 | 1.00 | 33.80 |
| | 5015 | C | ASN | 540 | 131.355 | 38.498 | 46.749 | 1.00 | 34.25 |
| | 5016 | O | ASN | 540 | 132.298 | 38.166 | 46.065 | 1.00 | 33.46 |
| | 5017 | CB | ASN | 540 | 131.047 | 37.127 | 48.775 | 1.00 | 33.03 |
| 35 | 5018 | CG | ASN | 540 | 131.463 | 36.902 | 50.198 | 1.00 | 39.77 |
| | 5019 | OD1 | ASN | 540 | 130.776 | 36.219 | 50.965 | 1.00 | 45.10 |
| | 5020 | ND2 | ASN | 540 | 132.581 | 37.502 | 50.579 | 1.00 | 36.91 |
| | 5021 | H | ASN | 540 | 129.781 | 39.280 | 49.311 | 1.00 | 25.00 |
| | 5022 | 1HD2 | ASN | 540 | 132.850 | 37.386 | 51.503 | 1.00 | 25.00 |
| 40 | 5023 | 2HD2 | ASN | 540 | 133.079 | 38.025 | 49.919 | 1.00 | 25.00 |
| | 5024 | N | LEU | 541 | 130.185 | 38.821 | 46.253 | 1.00 | 30.66 |
| | 5025 | CA | LEU | 541 | 129.997 | 38.848 | 44.821 | 1.00 | 31.93 |
| | 5026 | C | LEU | 541 | 130.262 | 40.166 | 44.110 | 1.00 | 33.86 |
| | 5027 | O | LEU | 541 | 130.805 | 40.129 | 42.977 | 1.00 | 30.07 |
| 45 | 5028 | CB | LEU | 541 | 128.600 | 38.308 | 44.486 | 1.00 | 34.62 |
| | 5029 | CG | LEU | 541 | 128.194 | 36.907 | 44.990 | 1.00 | 35.64 |
| | 5030 | CD1 | LEU | 541 | 126.882 | 36.542 | 44.345 | 1.00 | 31.26 |
| | 5031 | CD2 | LEU | 541 | 129.256 | 35.866 | 44.669 | 1.00 | 29.53 |
| | 5032 | H | LEU | 541 | 129.518 | 38.998 | 46.982 | 1.00 | 25.00 |
| 50 | 5033 | N | LEU | 542 | 129.910 | 41.305 | 44.706 | 1.00 | 35.33 |
| | 5034 | CA | LEU | 542 | 130.075 | 42.581 | 44.033 | 1.00 | 39.16 |
| | 5035 | C | LEU | 542 | 131.084 | 43.566 | 44.635 | 1.00 | 42.69 |

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|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 5036 | O | LEU | 542 | 131.361 | 44.614 | 44.055 | 1.00 | 45.28 |
| | 5037 | CB | LEU | 542 | 128.721 | 43.258 | 43.921 | 1.00 | 37.88 |
| | 5038 | CG | LEU | 542 | 127.685 | 42.494 | 43.105 | 1.00 | 37.82 |
| | 5039 | CD1 | LEU | 542 | 126.275 | 42.902 | 43.505 | 1.00 | 37.78 |
| 5 | 5040 | CD2 | LEU | 542 | 127.947 | 42.728 | 41.619 | 1.00 | 33.54 |
| | 5041 | H | LEU | 542 | 129.525 | 41.317 | 45.569 | 1.00 | 25.00 |
| | 5042 | N | VAL | 543 | 131.590 | 43.264 | 45.822 | 1.00 | 40.06 |
| | 5043 | CA | VAL | 543 | 132.536 | 44.167 | 46.483 | 1.00 | 39.62 |
| | 5044 | C | VAL | 543 | 133.960 | 43.601 | 46.457 | 1.00 | 40.35 |
| 10 | 5045 | O | VAL | 543 | 134.834 | 44.117 | 45.766 | 1.00 | 36.40 |
| | 5046 | CB | VAL | 543 | 132.112 | 44.458 | 47.951 | 1.00 | 38.67 |
| | 5047 | CG1 | VAL | 543 | 133.154 | 45.323 | 48.643 | 1.00 | 41.60 |
| | 5048 | CG2 | VAL | 543 | 130.762 | 45.137 | 47.966 | 1.00 | 33.55 |
| | 5049 | H | VAL | 543 | 131.348 | 42.421 | 46.245 | 1.00 | 25.00 |
| 15 | 5050 | N | ASP | 544 | 134.175 | 42.518 | 47.191 | 1.00 | 39.19 |
| | 5051 | CA | ASP | 544 | 135.485 | 41.887 | 47.274 | 1.00 | 37.12 |
| | 5052 | C | ASP | 544 | 135.802 | 40.970 | 46.112 | 1.00 | 38.65 |
| | 5053 | O | ASP | 544 | 134.991 | 40.124 | 45.739 | 1.00 | 42.40 |
| | 5054 | CB | ASP | 544 | 135.609 | 41.070 | 48.566 | 1.00 | 37.00 |
| 20 | 5055 | CG | ASP | 544 | 135.384 | 41.894 | 49.812 | 1.00 | 42.35 |
| | 5056 | OD1 | ASP | 544 | 135.659 | 43.114 | 49.803 | 1.00 | 49.35 |
| | 5057 | OD2 | ASP | 544 | 134.933 | 41.304 | 50.813 | 1.00 | 50.35 |
| | 5058 | H | ASP | 544 | 133.427 | 42.119 | 47.665 | 1.00 | 25.00 |
| | 5059 | N | SER | 545 | 136.984 | 41.153 | 45.543 | 1.00 | 36.71 |
| 25 | 5060 | CA | SER | 545 | 137.444 | 40.303 | 44.464 | 1.00 | 39.73 |
| | 5061 | C | SER | 545 | 138.200 | 39.158 | 45.142 | 1.00 | 38.96 |
| | 5062 | O | SER | 545 | 138.585 | 39.269 | 46.310 | 1.00 | 40.93 |
| | 5063 | CB | SER | 545 | 138.379 | 41.084 | 43.540 | 1.00 | 43.38 |
| | 5064 | OG | SER | 545 | 139.362 | 41.790 | 44.280 | 1.00 | 51.44 |
| 30 | 5065 | H | SER | 545 | 137.544 | 41.896 | 45.832 | 1.00 | 25.00 |
| | 5066 | HG | SER | 545 | 139.870 | 41.166 | 44.808 | 1.00 | 25.00 |
| | 5067 | N | ILE | 546 | 138.377 | 38.046 | 44.442 | 1.00 | 36.92 |
| | 5068 | CA | ILE | 546 | 139.109 | 36.920 | 45.011 | 1.00 | 40.59 |
| | 5069 | C | ILE | 546 | 140.602 | 37.261 | 44.954 | 1.00 | 45.93 |
| 35 | 5070 | O | ILE | 546 | 141.117 | 37.620 | 43.889 | 1.00 | 46.41 |
| | 5071 | CB | ILE | 546 | 138.839 | 35.612 | 44.226 | 1.00 | 36.34 |
| | 5072 | CG1 | ILE | 546 | 137.346 | 35.288 | 44.264 | 1.00 | 34.10 |
| | 5073 | CG2 | ILE | 546 | 139.629 | 34.456 | 44.829 | 1.00 | 31.04 |
| | 5074 | CD1 | ILE | 546 | 136.979 | 34.011 | 43.525 | 1.00 | 36.46 |
| 40 | 5075 | H | ILE | 546 | 138.009 | 37.990 | 43.533 | 1.00 | 25.00 |
| | 5076 | N | LYS | 547 | 141.282 | 37.201 | 46.009 | 1.00 | 52.49 |
| | 5077 | CA | LYS | 547 | 142.706 | 37.502 | 46.134 | 1.00 | 58.52 |
| | 5078 | C | LYS | 547 | 143.483 | 36.450 | 45.353 | 1.00 | 60.95 |
| | 5079 | O | LYS | 547 | 143.488 | 35.273 | 45.713 | 1.00 | 60.42 |
| 45 | 5080 | CB | LYS | 547 | 143.217 | 37.599 | 47.572 | 1.00 | 59.36 |
| | 5081 | CG | LYS | 547 | 144.684 | 38.023 | 47.659 | 1.00 | 68.28 |
| | 5082 | CD | LYS | 547 | 145.065 | 38.553 | 49.037 | 1.00 | 72.08 |
| | 5083 | CE | LYS | 547 | 146.486 | 39.105 | 49.029 | 1.00 | 74.86 |
| | 5084 | NZ | LYS | 547 | 146.796 | 39.880 | 50.265 | 1.00 | 78.47 |
| 50 | 5085 | H | LYS | 547 | 140.806 | 36.948 | 46.910 | 1.00 | 25.00 |
| | 5086 | 1HZ | LYS | 547 | 146.680 | 39.273 | 51.099 | 1.00 | 25.00 |
| | 5087 | 2HZ | LYS | 547 | 147.770 | 40.240 | 50.222 | 1.00 | 25.00 |

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|----|------|-----|-----|-----|---------|--------|--------|------|-------|
| | 5088 | 3HZ | LYS | 547 | 146.139 | 40.685 | 50.334 | 1.00 | 25.00 |
| | 5089 | N | ILE | 548 | 144.086 | 36.890 | 44.254 | 1.00 | 67.72 |
| | 5090 | CA | ILE | 548 | 144.868 | 36.018 | 43.381 | 1.00 | 76.79 |
| | 5091 | C | ILE | 548 | 146.198 | 35.622 | 44.025 | 1.00 | 83.68 |
| 5 | 5092 | O | ILE | 548 | 146.583 | 34.440 | 43.897 | 1.00 | 86.24 |
| | 5093 | CB | ILE | 548 | 145.120 | 36.678 | 41.986 | 1.00 | 75.68 |
| | 5094 | CG1 | ILE | 548 | 145.604 | 38.125 | 42.152 | 1.00 | 78.47 |
| | 5095 | CG2 | ILE | 548 | 143.855 | 36.623 | 41.137 | 1.00 | 68.49 |
| | 5096 | CD1 | ILE | 548 | 145.930 | 38.827 | 40.831 | 1.00 | 78.93 |
| 10 | 5097 | OXT | ILE | 548 | 146.823 | 36.492 | 44.672 | 1.00 | 92.78 |
| | 5098 | H | ILE | 548 | 144.032 | 37.836 | 44.045 | 1.00 | 25.00 |
| | 5099 | ILE | 548 | | | | | | |
| | 5100 | MG | MG | 851 | 104.185 | 36.235 | 53.030 | 1.00 | 61.83 |
| | 5101 | MG | MG | 852 | 102.138 | 43.657 | 49.009 | 1.00 | 62.23 |
| 15 | 5102 | O | HOH | 601 | 107.742 | 22.057 | 32.406 | 1.00 | 15.11 |
| | 5103 | O | HOH | 602 | 122.540 | 22.695 | 37.531 | 1.00 | 32.44 |
| | 5104 | O | HOH | 603 | 127.188 | 14.109 | 43.835 | 1.00 | 23.85 |
| | 5105 | O | HOH | 604 | 123.257 | 32.177 | 37.651 | 1.00 | 25.21 |
| | 5106 | O | HOH | 605 | 131.975 | 36.814 | 38.945 | 1.00 | 20.08 |
| 20 | 5107 | O | HOH | 606 | 130.320 | 38.579 | 40.729 | 1.00 | 28.69 |
| | 5108 | O | HOH | 607 | 124.735 | 33.181 | 39.810 | 1.00 | 19.46 |
| | 5109 | O | HOH | 608 | 119.958 | 22.714 | 50.725 | 1.00 | 24.82 |
| | 5110 | O | HOH | 609 | 125.172 | 22.654 | 40.253 | 1.00 | 21.47 |
| | 5111 | O | HOH | 610 | 106.047 | 21.994 | 29.826 | 1.00 | 26.03 |
| 25 | 5112 | O | HOH | 611 | 123.659 | 29.782 | 47.444 | 1.00 | 22.10 |
| | 5113 | O | HOH | 612 | 129.924 | 22.165 | 49.955 | 1.00 | 20.33 |
| | 5114 | O | HOH | 613 | 117.254 | 16.672 | 36.732 | 1.00 | 18.88 |
| | 5115 | O | HOH | 614 | 131.911 | 22.935 | 48.204 | 1.00 | 23.59 |
| | 5116 | O | HOH | 615 | 123.421 | 30.030 | 35.911 | 1.00 | 23.89 |
| 30 | 5117 | O | HOH | 616 | 128.952 | 30.316 | 38.829 | 1.00 | 22.41 |
| | 5118 | O | HOH | 617 | 98.347 | 33.326 | 40.948 | 1.00 | 28.07 |
| | 5119 | O | HOH | 618 | 126.062 | 19.250 | 36.922 | 1.00 | 29.11 |
| | 5120 | O | HOH | 619 | 133.788 | 33.099 | 36.415 | 1.00 | 20.10 |
| | 5121 | O | HOH | 620 | 127.252 | 22.013 | 48.848 | 1.00 | 24.10 |
| 35 | 5122 | O | HOH | 621 | 123.122 | 19.043 | 45.472 | 1.00 | 19.68 |
| | 5123 | O | HOH | 622 | 124.636 | 25.767 | 41.845 | 1.00 | 42.37 |
| | 5124 | O | HOH | 623 | 138.021 | 26.937 | 54.497 | 1.00 | 33.32 |
| | 5125 | O | HOH | 624 | 130.604 | 16.213 | 44.273 | 1.00 | 25.46 |
| | 5126 | O | HOH | 625 | 119.735 | 17.425 | 55.175 | 1.00 | 23.51 |
| 40 | 5127 | O | HOH | 626 | 109.560 | 43.332 | 32.386 | 1.00 | 27.79 |
| | 5128 | O | HOH | 627 | 104.016 | 36.817 | 39.018 | 1.00 | 24.34 |
| | 5129 | O | HOH | 628 | 134.051 | 35.256 | 29.604 | 1.00 | 37.22 |
| | 5130 | O | HOH | 629 | 107.947 | 18.792 | 36.023 | 1.00 | 35.84 |
| | 5131 | O | HOH | 630 | 129.821 | 19.576 | 48.096 | 1.00 | 29.63 |
| 45 | 5132 | O | HOH | 631 | 104.550 | 21.758 | 41.675 | 1.00 | 38.10 |
| | 5133 | O | HOH | 632 | 111.970 | 10.709 | 47.161 | 1.00 | 23.86 |
| | 5134 | O | HOH | 633 | 125.976 | 29.448 | 50.341 | 1.00 | 26.42 |
| | 5135 | O | HOH | 634 | 97.143 | 36.787 | 48.102 | 1.00 | 35.12 |
| | 5136 | O | HOH | 635 | 121.582 | 36.805 | 25.111 | 1.00 | 35.51 |
| 50 | 5137 | O | HOH | 636 | 113.756 | 26.801 | 22.571 | 1.00 | 30.58 |
| | 5138 | O | HOH | 637 | 124.698 | 19.485 | 28.803 | 1.00 | 29.60 |
| | 5139 | O | HOH | 638 | 130.563 | 25.567 | 43.476 | 1.00 | 29.93 |

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|----|------|---|-----|------|---------|--------|--------|------|-------|
| | 5140 | O | HOH | 639 | 121.706 | 39.646 | 27.124 | 1.00 | 32.61 |
| | 5141 | O | HOH | 640 | 104.749 | 34.099 | 30.683 | 1.00 | 28.14 |
| | 5142 | O | HOH | 641 | 111.751 | 8.174 | 35.080 | 1.00 | 34.23 |
| | 5143 | O | HOH | 642 | 120.339 | 31.400 | 41.487 | 1.00 | 52.69 |
| 5 | 5144 | O | HOH | 643 | 95.163 | 26.623 | 43.384 | 1.00 | 36.83 |
| | 5145 | O | HOH | 644 | 137.113 | 41.980 | 40.124 | 1.00 | 30.35 |
| | 5146 | O | HOH | 645 | 116.126 | 11.318 | 49.986 | 1.00 | 25.34 |
| | 5147 | O | HOH | 646 | 110.165 | 35.328 | 17.495 | 1.00 | 37.81 |
| | 5148 | O | HOH | 647 | 118.054 | 20.287 | 30.749 | 1.00 | 33.12 |
| 10 | 5149 | O | HOH | 648 | 115.899 | 40.354 | 30.351 | 1.00 | 29.82 |
| | 5150 | O | HOH | 649 | 113.524 | 54.000 | 32.295 | 1.00 | 30.14 |
| | 5151 | O | HOH | 650 | 127.950 | 27.982 | 37.184 | 1.00 | 28.39 |
| | 5152 | O | HOH | 651 | 108.770 | 18.109 | 30.127 | 1.00 | 36.94 |
| | 5153 | O | HOH | 652 | 112.843 | 23.036 | 50.160 | 1.00 | 41.87 |
| 15 | 5154 | O | HOH | 653 | 132.804 | 32.747 | 50.167 | 1.00 | 34.56 |
| | 5155 | O | HOH | 654 | 99.278 | 32.670 | 36.214 | 1.00 | 31.88 |
| | 5156 | O | HOH | 655 | 93.100 | 36.093 | 41.777 | 1.00 | 39.13 |
| | 5157 | O | HOH | 656 | 114.575 | 17.087 | 50.058 | 1.00 | 29.96 |
| | 5158 | O | HOH | 657 | 134.890 | 18.651 | 45.599 | 1.00 | 29.79 |
| 20 | 5159 | O | HOH | 658 | 134.764 | 16.354 | 47.235 | 1.00 | 41.87 |
| | 5160 | O | HOH | 659 | 138.146 | 19.452 | 46.210 | 1.00 | 40.62 |
| | 5161 | O | HOH | 660 | 113.498 | 7.243 | 37.601 | 1.00 | 44.14 |
| | 5162 | O | HOH | 661 | 118.735 | 25.324 | 49.539 | 1.00 | 32.46 |
| | 5163 | O | HOH | 662 | 121.072 | 19.323 | 57.037 | 1.00 | 28.13 |
| 25 | 5164 | O | HOH | 663 | 120.647 | 52.139 | 31.726 | 1.00 | 31.21 |
| | 5165 | O | HOH | 664 | 125.201 | 27.805 | 35.886 | 1.00 | 35.41 |
| | 5166 | O | HOH | 665 | 103.040 | 17.910 | 41.249 | 1.00 | 34.74 |
| | 5167 | O | HOH | 666 | 92.281 | 23.719 | 49.317 | 1.00 | 36.36 |
| | 5168 | O | HOH | 667 | 120.731 | 30.312 | 30.736 | 1.00 | 40.91 |
| 30 | 5169 | O | HOH | 668 | 111.010 | 16.805 | 31.260 | 1.00 | 37.18 |
| | 5170 | O | HOH | 669 | 98.374 | 30.892 | 39.496 | 1.00 | 39.09 |
| | 5171 | O | HOH | 670 | 142.913 | 20.086 | 59.043 | 1.00 | 40.89 |
| | 5172 | O | HOH | 671 | 120.070 | 4.238 | 32.203 | 1.00 | 32.10 |
| | 5173 | O | HOH | 672 | 116.885 | 14.360 | 38.230 | 1.00 | 19.20 |
| 35 | 5174 | O | HOH | 673 | 135.198 | 31.364 | 38.159 | 1.00 | 21.99 |
| | 5175 | O | HOH | 674 | 130.652 | 23.815 | 45.653 | 1.00 | 22.37 |
| | 5176 | O | HOH | 675 | 116.184 | 18.170 | 25.042 | 1.00 | 33.65 |
| | 5177 | O | HOH | 676 | 102.763 | 37.505 | 36.535 | 1.00 | 29.50 |
| | 5178 | O | HOH | 677 | 113.482 | 17.709 | 47.318 | 1.00 | 24.10 |
| 40 | 5179 | O | HOH | 678 | 128.292 | 24.082 | 47.295 | 1.00 | 27.62 |
| | 5180 | O | HOH | 679 | 128.934 | 20.011 | 39.747 | 1.00 | 26.34 |
| | 5181 | O | HOH | 680 | 129.840 | 32.556 | 48.799 | 1.00 | 34.07 |
| | 5182 | O | HOH | 681 | 115.123 | 17.894 | 45.342 | 1.00 | 23.02 |
| | 5183 | O | HOH | 682 | 134.875 | 11.928 | 61.810 | 1.00 | 24.68 |
| 45 | 5184 | O | HOH | 683 | 140.837 | 17.873 | 38.782 | 1.00 | 33.65 |
| | 5185 | O | HOH | 684 | 135.724 | 8.315 | 55.152 | 1.00 | 37.93 |
| | 5186 | O | HOH | 685 | 131.660 | 25.765 | 56.520 | 1.00 | 36.71 |
| | 5187 | O | HOH | 686 | 148.447 | 27.966 | 42.675 | 1.00 | 38.11 |
| | 5188 | O | HOH | 687 | 110.190 | 10.176 | 45.195 | 1.00 | 35.74 |
| 50 | 5189 | O | HOH | 688 | 109.091 | 17.883 | 25.410 | 1.00 | 38.94 |
| | 5190 | O | HOH | 6889 | 104.860 | 34.526 | 28.030 | 1.00 | 38.81 |
| | 5191 | O | HOH | 690 | 102.070 | 36.177 | 27.889 | 1.00 | 35.60 |

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|----|------|---|-----|-----|---------|---------|--------|------|-------|
| | 5192 | O | HOH | 691 | 118.113 | 11.174 | 28.782 | 1.00 | 38.94 |
| | 5193 | O | HOH | 692 | 131.635 | 20.640 | 62.725 | 1.00 | 33.60 |
| | 5194 | O | HOH | 693 | 136.344 | 35.530 | 31.124 | 1.00 | 36.08 |
| | 5195 | O | HOH | 694 | 120.257 | 31.406 | 33.335 | 1.00 | 31.14 |
| 5 | 5196 | O | HOH | 695 | 102.005 | 32.616 | 56.124 | 1.00 | 33.30 |
| | 5197 | O | HOH | 696 | 124.575 | 21.994 | 35.468 | 1.00 | 36.59 |
| | 5198 | O | HOH | 697 | 101.923 | 20.169 | 46.398 | 1.00 | 40.37 |
| | 5199 | O | HOH | 698 | 129.243 | 49.171 | 40.765 | 1.00 | 49.17 |
| | 5200 | O | HOH | 699 | 139.196 | 35.578 | 48.616 | 1.00 | 31.26 |
| 10 | 5201 | O | HOH | 700 | 134.064 | 15.022 | 43.146 | 1.00 | 40.48 |
| | 5202 | O | HOH | 701 | 128.514 | 31.051 | 51.675 | 1.00 | 39.32 |
| | 5203 | O | HOH | 702 | 112.958 | 10.222 | 36.694 | 1.00 | 47.07 |
| | 5204 | O | HOH | 703 | 109.649 | 15.841 | 28.459 | 1.00 | 35.43 |
| | 5205 | O | HOH | 704 | 140.094 | 42.685 | 39.958 | 1.00 | 41.31 |
| 15 | 5206 | O | HOH | 705 | 86.608 | 31.749 | 55.350 | 1.00 | 36.82 |
| | 5207 | O | HOH | 706 | 128.605 | 34.147 | 28.351 | 1.00 | 35.79 |
| | 5208 | O | HOH | 707 | 87.075 | 34.369 | 56.433 | 1.00 | 42.04 |
| | 5209 | O | HOH | 708 | 89.030 | 34.345 | 44.620 | 1.00 | 40.07 |
| | 5210 | O | HOH | 709 | 104.535 | 51.407 | 27.998 | 1.00 | 39.44 |
| 20 | 5211 | O | HOH | 710 | 120.125 | 34.187 | 24.397 | 1.00 | 63.74 |
| | 5212 | O | HOH | 711 | 100.184 | 37.778 | 52.580 | 1.00 | 43.18 |
| | 5213 | O | HOH | 712 | 109.218 | 37.444 | 46.111 | 1.00 | 37.68 |
| | 5214 | O | HOH | 713 | 139.550 | 20.401 | 60.539 | 1.00 | 40.82 |
| | 5215 | O | HOH | 714 | 140.612 | 17.7933 | 52.684 | 1.00 | 42.33 |
| 25 | 5216 | O | HOH | 715 | 120.330 | 21.170 | 32.392 | 1.00 | 31.20 |
| | 5217 | O | HOH | 716 | 100.372 | 35.917 | 30.033 | 1.00 | 43.22 |
| | 5218 | O | HOH | 717 | 120.163 | 23.899 | 33.930 | 1.00 | 33.67 |
| | 5219 | O | HOH | 718 | 146.383 | 28.556 | 40.921 | 1.00 | 38.01 |
| | 5220 | O | HOH | 719 | 109.966 | 20.788 | 31.041 | 1.00 | 38.62 |
| 30 | 5221 | O | HOH | 720 | 105.493 | 40.925 | 45.887 | 1.00 | 35.53 |
| | 5222 | O | HOH | 721 | 119.171 | 27.937 | 23.152 | 1.00 | 55.39 |
| | 5223 | O | HOH | 722 | 124.424 | 41.390 | 25.938 | 1.00 | 43.52 |
| | 5224 | O | HOH | 723 | 102.779 | 17.993 | 48.134 | 1.00 | 38.38 |
| | 5225 | O | HOH | 724 | 112.387 | 5.685 | 33.453 | 1.00 | 48.35 |
| 35 | 5226 | O | HOH | 725 | 151.082 | 25.140 | 44.349 | 1.00 | 35.50 |
| | 5227 | O | HOH | 726 | 127.089 | 21.203 | 29.049 | 1.00 | 45.21 |
| | 5228 | O | HOH | 727 | 133.178 | 5.551 | 47.734 | 1.00 | 39.38 |
| | 5229 | O | HOH | 728 | 151.127 | 34.628 | 33.927 | 1.00 | 42.02 |
| | 5230 | O | HOH | 729 | 150.405 | 22.240 | 44.559 | 1.00 | 38.43 |
| 40 | 5231 | O | HOH | 730 | 131.660 | 2.107 | 47.933 | 1.00 | 37.78 |
| | 5232 | O | HOH | 731 | 135.465 | 8.584 | 52.047 | 1.00 | 40.15 |
| | 5233 | O | HOH | 732 | 147.814 | 29.664 | 45.229 | 1.00 | 44.50 |
| | 5234 | O | HOH | 733 | 140.989 | 33.094 | 47.707 | 1.00 | 43.19 |
| | 5235 | O | HOH | 734 | 103.951 | 49.441 | 25.596 | 1.00 | 38.72 |
| 45 | 5236 | O | HOH | 735 | 86.471 | 53.747 | 29.731 | 1.00 | 43.56 |
| | 5237 | O | HOH | 736 | 134.470 | 31.168 | 25.546 | 1.00 | 52.39 |
| | 5238 | O | HOH | 737 | 122.918 | 25.464 | 36.469 | 1.00 | 42.39 |
| | 5239 | O | HOH | 738 | 99.309 | 33.456 | 31.178 | 1.00 | 48.32 |
| | 5240 | O | HOH | 739 | 91.548 | 47.290 | 47.278 | 1.00 | 45.43 |
| 50 | 5241 | O | HOH | 740 | 92.024 | 43.380 | 40.690 | 1.00 | 42.02 |
| | 5242 | O | HOH | 741 | 149.190 | 38.195 | 52.530 | 1.00 | 47.74 |
| | 5243 | O | HOH | 742 | 153.088 | 41.575 | 36.804 | 1.00 | 46.51 |

| | | | | | | | | | |
|----|------|---|-----|-----|----------|--------|--------|------|-------|
| | 5244 | O | HOH | 743 | 138.714 | 31.651 | 53.657 | 1.00 | 43.64 |
| | 5245 | O | HOH | 744 | 143.900 | 19.054 | 51.722 | 1.00 | 40.32 |
| | 5246 | O | HOH | 745 | 138.795 | 15.536 | 49.608 | 1.00 | 43.79 |
| | 5247 | O | HOH | 746 | 124.711 | -3.430 | 56.077 | 1.00 | 44.40 |
| 5 | 5248 | O | HOH | 747 | 145.969 | 30.921 | 42.825 | 1.00 | 39.08 |
| | 5249 | O | HOH | 748 | 134.979 | 10.249 | 59.470 | 1.00 | 35.78 |
| | 5250 | O | HOH | 749 | 133.932 | 40.151 | 29.911 | 1.00 | 41.40 |
| | 5251 | O | HOH | 750 | 114.521 | 21.309 | 22.697 | 1.00 | 38.72 |
| | 5252 | O | HOH | 751 | 129.614 | 38.180 | 25.426 | 1.00 | 39.89 |
| 10 | 5253 | O | HOH | 752 | 111.6443 | 13.087 | 29.735 | 1.00 | 45.90 |
| | 5254 | O | HOH | 753 | 104.216 | 21.388 | 44.848 | 1.00 | 33.35 |
| | 5255 | O | HOH | 754 | 110.986 | 12.520 | 49.459 | 1.00 | 49.32 |
| | 5256 | O | HOH | 755 | 139.600 | 40.725 | 48.728 | 1.00 | 46.07 |
| | 5257 | O | HOH | 756 | 113.295 | 9.448 | 29.832 | 1.00 | 35.78 |
| 15 | 5258 | O | HOH | 757 | 127.101 | 23.382 | 34.156 | 1.00 | 48.02 |
| | 5259 | O | HOH | 758 | 127.933 | 18.490 | 63.251 | 1.00 | 46.33 |
| | 5260 | O | HOH | 759 | 130.420 | 26.867 | 25.702 | 1.00 | 40.40 |
| | 5261 | O | HOH | 760 | 122.231 | 3.237 | 35.918 | 1.00 | 44.61 |
| | 5262 | O | HOH | 761 | 128.310 | 26.484 | 40.968 | 1.00 | 32.14 |
| 20 | 5263 | O | HOH | 762 | 88.443 | 24.530 | 48.586 | 1.00 | 57.07 |
| | 5264 | O | HOH | 763 | 103.542 | 23.739 | 25.080 | 1.00 | 45.05 |
| | 5265 | O | HOH | 764 | 116.278 | 57.331 | 34.559 | 1.00 | 42.40 |
| | 5266 | O | HOH | 765 | 120.787 | 5.886 | 61.156 | 1.00 | 43.73 |
| | 5267 | O | HOH | 766 | 142.631 | 40.352 | 42.775 | 1.00 | 65.94 |
| 25 | 5268 | O | HOH | 767 | 124.244 | 13.057 | 63.666 | 1.00 | 43.68 |
| | 5269 | O | HOH | 768 | 101.830 | 22.900 | 29.735 | 1.00 | 36.47 |
| | 5270 | O | HOH | 769 | 137.190 | 5.022 | 37.071 | 1.00 | 50.65 |
| | 5271 | O | HOH | 770 | 135.078 | 34.403 | 50.639 | 1.00 | 51.53 |
| | 5272 | O | HOH | 771 | 103.266 | 58.719 | 26.225 | 1.00 | 46.58 |
| 30 | 5273 | O | HOH | 772 | 144.319 | 16.861 | 24.565 | 1.00 | 53.32 |
| | 5274 | O | HOH | 773 | 127.856 | 47.718 | 31.019 | 1.00 | 45.45 |
| | 5275 | O | HOH | 774 | 95.530 | 18.110 | 49.546 | 1.00 | 52.47 |
| | 5276 | O | HOH | 775 | 148.435 | 20.165 | 43.831 | 1.00 | 49.25 |
| | 5277 | O | HOH | 776 | 118.026 | 13.535 | 59.021 | 1.00 | 48.41 |
| 35 | 5278 | O | HOH | 777 | 110.119 | 43.903 | 16.201 | 1.00 | 37.10 |
| | 5279 | O | HOH | 778 | 110.457 | 61.356 | 39.879 | 1.00 | 44.66 |
| | 5280 | O | HOH | 779 | 105.313 | 56.879 | 27.692 | 1.00 | 51.08 |
| | 5281 | O | HOH | 780 | 106.267 | 19.656 | 28.049 | 1.00 | 45.55 |
| | 5282 | O | HOH | 781 | 122.226 | 20.789 | 29.638 | 1.00 | 45.73 |
| 40 | 5283 | O | HOH | 782 | 107.680 | 19.165 | 33.248 | 1.00 | 35.37 |
| | 5284 | O | HOH | 783 | 141.434 | 30.527 | 58.190 | 1.00 | 56.49 |
| | 5285 | O | HOH | 784 | 121.953 | 27.180 | 30.544 | 1.00 | 43.22 |
| | 5286 | O | HOH | 785 | 116.050 | 27.492 | 52.913 | 1.00 | 59.86 |
| | 5287 | O | HOH | 786 | 115.271 | 11.494 | 53.629 | 1.00 | 47.46 |
| 45 | 5288 | O | HOH | 787 | 136.166 | 43.700 | 43.430 | 1.00 | 44.89 |
| | 5289 | O | HOH | 788 | 123.135 | 5.923 | 32.296 | 1.00 | 61.24 |
| | 5290 | O | HOH | 789 | 148.342 | 38.089 | 38.232 | 1.00 | 41.22 |
| | 5291 | O | HOH | 790 | 112.195 | 39.980 | 44.065 | 1.00 | 44.26 |
| | 5292 | O | HOH | 791 | 108.340 | 50.773 | 20.100 | 1.00 | 62.55 |
| 50 | 5293 | O | HOH | 792 | 126.140 | 29.670 | 29.775 | 1.00 | 38.87 |
| | 5294 | O | HOH | 793 | 122.347 | 26.176 | 27.904 | 1.00 | 47.43 |
| | 5295 | O | HOH | 794 | 105.375 | 13.283 | 37.860 | 1.00 | 40.63 |

| | | | | | | | | | |
|----|------|---|-----|-----|---------|--------|---------|------|-------|
| | 5296 | O | HOH | 795 | 146.608 | 19.061 | 33.529 | 1.00 | 50.53 |
| | 5297 | O | HOH | 796 | 112.240 | 28.192 | 56.028 | 1.00 | 54.08 |
| | 5298 | O | HOH | 797 | 106.519 | 16.717 | 37.160 | 1.00 | 39.17 |
| | 5299 | O | HOH | 798 | 122.257 | -2.147 | 57.632 | 1.00 | 59.87 |
| 5 | 5300 | O | HOH | 799 | 105.969 | 47.469 | 20.174 | 1.00 | 42.44 |
| | 5301 | O | HOH | 800 | 124.201 | 23.387 | 29.951 | 1.00 | 51.85 |
| | 5302 | O | HOH | 801 | 104.010 | 26.139 | 23.199 | 1.00 | 57.02 |
| | 5303 | O | HOH | 802 | 106.547 | 37.540 | 47.839 | 1.00 | 46.00 |
| | 5304 | O | HOH | 803 | 126.083 | 27.795 | 33.246 | 1.00 | 45.66 |
| 10 | 5305 | O | HOH | 804 | 93.229 | 25.530 | 63.301 | 1.00 | 50.45 |
| | 5306 | O | HOH | 805 | 126.637 | 14.627 | 66.291 | 1.00 | 54.63 |
| | 5307 | O | HOH | 806 | 117.649 | 48.031 | 30.248 | 1.00 | 44.41 |
| | 5308 | O | HOH | 807 | 112.889 | 34.483 | 46.820 | 1.00 | 41.77 |
| | 5309 | O | HOH | 808 | 143.749 | 8.474 | 39.051 | 1.00 | 58.35 |
| 15 | 5310 | O | HOH | 809 | 117.223 | 16.467 | 56.527 | 1.00 | 54.55 |
| | 5311 | O | HOH | 810 | 136.640 | 48.794 | 42.640 | 1.00 | 59.70 |
| | 5312 | O | HOH | 811 | 130.573 | 47.631 | 52.219 | 1.00 | 43.65 |
| | 5313 | O | HOH | 812 | 119.790 | 22.620 | 53.732 | 1.00 | 49.88 |
| | 5314 | O | HOH | 813 | 105.220 | 9.911 | 43.334 | 1.00 | 53.82 |
| 20 | 5315 | O | HOH | 814 | 94.459 | 22.230 | 65.891 | 1.00 | 53.43 |
| | 5316 | O | HOH | 815 | 145.893 | 33.119 | 447.904 | 1.00 | 50.15 |
| | 5317 | O | HOH | 816 | 137.540 | 19.003 | 49.581 | 1.00 | 32.04 |
| | 5318 | O | HOH | 817 | 127.395 | 18.676 | 22.177 | 1.00 | 58.02 |
| | 5319 | O | HOH | 818 | 135.930 | 19.361 | 20.695 | 1.00 | 61.65 |
| 25 | 5320 | O | HOH | 819 | 122.368 | -4.865 | 43.028 | 1.00 | 43.72 |
| | 5321 | O | HOH | 820 | 117.352 | 52.131 | 24.538 | 1.00 | 49.67 |
| | 5322 | O | HOH | 821 | 129.874 | 51.577 | 33.814 | 1.00 | 58.12 |
| | 5323 | O | HOH | 822 | 129.360 | 28.179 | 34.594 | 1.00 | 43.67 |
| | 5324 | O | HOH | 823 | 97.243 | 40.051 | 31.308 | 1.00 | 40.94 |
| 30 | 5325 | O | HOH | 824 | 119.361 | 23.189 | 24.691 | 1.00 | 55.59 |
| | 5326 | O | HOH | 825 | 105.947 | 8.433 | 39.961 | 1.00 | 47.78 |
| | 5327 | O | HOH | 826 | 124.177 | -6.929 | 48.285 | 1.00 | 50.47 |
| | 5328 | O | HOH | 827 | 143.743 | 41.219 | 49.977 | 1.00 | 54.42 |
| | 5329 | O | HOH | 828 | 117.815 | 15.765 | 23.926 | 1.00 | 47.10 |
| 35 | 5330 | O | HOH | 829 | 106.852 | 11.509 | 45.366 | 1.00 | 59.91 |
| | 5331 | O | HOH | 830 | 114.340 | 49.442 | 45.031 | 1.00 | 54.21 |
| | 5332 | O | HOH | 831 | 107.212 | 10.319 | 38.018 | 1.00 | 47.91 |
| | 5333 | O | HOH | 832 | 89.843 | 54.539 | 37.711 | 1.00 | 55.79 |
| | 5334 | O | HOH | 833 | 115.120 | 21.415 | 49.941 | 1.00 | 40.64 |
| 40 | 5335 | O | HOH | 834 | 119.324 | 14.942 | 62.472 | 1.00 | 63.27 |
| | 5336 | O | HOH | 835 | 149.479 | 14.241 | 50.723 | 1.00 | 65.18 |
| | 5337 | O | HOH | 836 | 99.208 | 46.311 | 26.331 | 1.00 | 59.48 |
| | 5338 | O | HOH | 837 | 146.479 | 34.108 | 25.046 | 1.00 | 49.79 |
| | 5339 | O | HOH | 838 | 117.731 | 49.616 | 19.065 | 1.00 | 60.65 |
| 45 | 5340 | O | HOH | 839 | 115.539 | 6.301 | 34.276 | 1.00 | 51.97 |
| | 5341 | O | HOH | 840 | 97.213 | 27.831 | 34.233 | 1.00 | 45.30 |
| | 5342 | O | HOH | 841 | 89.788 | 22.728 | 43.919 | 1.00 | 61.79 |
| | 5343 | O | HOH | 842 | 147.830 | 32.323 | 40.885 | 1.00 | 46.95 |
| | 5344 | O | HOH | 843 | 132.462 | 17.381 | 68.762 | 1.00 | 50.53 |
| 50 | 5345 | O | HOH | 844 | 140.816 | 13.261 | 39.613 | 1.00 | 50.48 |
| | 5346 | O | HOH | 845 | 131.788 | 48.689 | 43.107 | 1.00 | 55.44 |
| | 5347 | O | HOH | 846 | 106.451 | 38.430 | 52.704 | 1.00 | 44.59 |

| | | | | | | | | | |
|----|------|---|-----|-----|---------|--------|--------|------|-------|
| | 5348 | O | HOH | 847 | 112.522 | 3.225 | 51.067 | 1.00 | 62.24 |
| | 5349 | O | HOH | 848 | 116.588 | 33.059 | 17.286 | 1.00 | 51.54 |
| | 5350 | O | HOH | 849 | 121.984 | 13.530 | 21.831 | 1.00 | 59.69 |
| | 5351 | O | HOH | 850 | 121.351 | 34.646 | 19.580 | 1.00 | 63.69 |
| 5 | 5352 | O | HOH | 853 | 119.444 | 26.300 | 52.657 | 1.00 | 48.12 |
| | 5353 | O | HOH | 854 | 119.223 | 18.972 | 28.280 | 1.00 | 43.53 |
| | 5354 | O | HOH | 855 | 109.476 | 29.077 | 61.498 | 1.00 | 46.95 |
| | 5355 | O | HOH | 856 | 96.378 | 36.846 | 50.773 | 1.00 | 37.88 |
| | 5356 | O | HOH | 857 | 96.918 | 46.467 | 51.605 | 1.00 | 69.73 |
| 10 | 5357 | O | HOH | 858 | 97.861 | 35.983 | 32.096 | 1.00 | 48.71 |
| | 5358 | O | HOH | 859 | 105.582 | 44.217 | 22.626 | 1.00 | 52.96 |
| | 5359 | O | HOH | 860 | 111.207 | 54.577 | 33.852 | 1.00 | 44.86 |
| | 5360 | O | HOH | 861 | 106.475 | 45.773 | 50.620 | 1.00 | 52.70 |
| | 5361 | O | HOH | 862 | 136.750 | 45.222 | 40.123 | 1.00 | 53.92 |
| 15 | 5362 | O | HOH | 863 | 134.438 | 43.600 | 31.414 | 1.00 | 51.51 |
| | 5363 | O | HOH | 864 | 147.130 | 24.676 | 49.884 | 1.00 | 42.49 |
| | 5364 | O | HOH | 865 | 126.425 | 22.757 | 59.405 | 1.00 | 54.25 |
| | 5365 | O | HOH | 866 | 135.514 | 7.098 | 48.245 | 1.00 | 59.13 |
| | 5366 | O | HOH | 867 | 114.942 | 1.622 | 48.125 | 1.00 | 56.08 |
| 20 | 5367 | O | HOH | 868 | 119.740 | -4.108 | 46.312 | 1.00 | 51.35 |
| | 5368 | O | HOH | 869 | 134.478 | 8.308 | 29.219 | 1.00 | 53.23 |
| | 5369 | O | HOH | 870 | 127.297 | 14.232 | 21.009 | 1.00 | 54.19 |
| | 5370 | O | HOH | 871 | 134.315 | 17.294 | 22.547 | 1.00 | 59.58 |
| | 5371 | O | HOH | 872 | 130.159 | 26.543 | 36.441 | 1.00 | 34.46 |
| 25 | 5372 | O | HOH | 873 | 136.207 | 18.694 | 43.344 | 1.00 | 35.20 |
| | 5373 | O | HOH | 874 | 134.779 | 10.368 | 41.428 | 1.00 | 45.81 |
| | 5374 | O | HOH | 875 | 137.054 | 3.899 | 33.453 | 1.00 | 51.47 |
| | 5375 | O | HOH | 876 | 145.762 | 17.318 | 28.638 | 1.00 | 52.42 |
| | 5376 | O | HOH | 877 | 146.344 | 20.944 | 29.342 | 1.00 | 47.62 |

TABLE 12

Score = 167 bits (419), Expect = 5e-41
 Identities = 88/270 (32%), Positives = 152/270 (55%), Gaps = 5/270 (1%)

Query: 1 DRVVECYFWALGVYFEPQYSQARVMLVKTISMISIVDDTFDAYGTVKELEYTDAIQPWD 60
 DR+VECYFW G+ Q++ AR+M+ K ++I+++DD +D YGT++ELE +TD I+RWD
 Sbjct: 316 DRLVECYFWNTGIIEPRQHASARIMMGKVNALITVIDDIYDVYGTLEELEQFTDLIRWD 375

Query: 61 INEIDRLPDYMKISYKAILDLYKDYEKELSSAGRSHIVCHAIERMKEVVRNYNVESTWFI 120
 IN ID+LPDYM++ + A+ + D ++ +++ + + ++ Y VE+ WF
 Sbjct: 376 INSIDQLPDYMLCFLALNNFVDDTSYDVMKEKGVNVIPYLRQSWVDLADKYMVEARWY 435

Query: 121 EGYMPPVSEYLSNALATTTYYLATTSYLGM-KSATEQDFEWLSKNPKILEASVIICRVI 179
 G+ P + EYL N+ + + + T + + S T++ + L K ++ S + R+
 Sbjct: 436 GGHKPSLEEYLENSWQSISGPCMLTHIFFRVTDSFTKETVDSLYKYHDLVRWSSFVLRLA 495

Query: 180 DDTATYEVEKSRGQIATGIECCMRDYGISTKEAMAKFQNMATAWKDIN-EGLLRPTPVS 238
 DD T E SRG + ++C M DY S EA + + WK +N E + + +P
 Sbjct: 496 DDLGTSVEEVSRGDVPKSLQCYMSDYNASEAEARKHVWKLIAEVWKKMNAERVSKDSPFG 555

Query: 239 TEFLTPILNLARIVEVTYIHNLDGY--THP 266
 +F+ ++L R+ ++ Y HN DG+ HP
 Sbjct: 556 KDFIGCAVDLGRMAQLMY-HNGDGHGTQHP 584

TABLE 13

Score = 116 bits (289), Expect = 1e-25
 Identities = 77/270 (28%), Positives = 126/270 (46%), Gaps = 6/270 (2%)

Query: 3 VAEVYFSSATFEP-EYSATRIAFTKIGCLQVLFDMDADIFATLDELKSFTEGVKRWDTSL 61
 V +++ FEP ++ R I L + DD+ D++ TLDEL+ FT+ KRWDT
 Sbjct: 318 VESFFWAVGMFEPHQHGYQRKMAATIIVLATVIDDIYDVYGTLDLELFTDTFKRWDTES 377

Query: 62 LHEIPECMQTCKVWFKLMEEVNNDVVKVQGRDMLAHIRKPWELYFNCYVQEREWLEAGY 121
 + +P MQ C+ + + D++K G L ++RK Y E +W +GY
 Sbjct: 378 ITRLPYMQLCYWGVDHNYISDAAYDILKEHGFFCLQYLRKSVVDLVEAYFHEAKWYHSGY 437

Query: 122 IPTFEEYLKTYAISVGLGPCTLQPIILLMGELVKDD--VVEKVHYPNSMFMELVSLSWRLTN 179
 P+ +EYL ISV P + P D V++ ++ ++ L + RL +
 Sbjct: 438 TPSLDEYLNIAKISVA-SPAIIISPTYFTFANASHDTAVIDSLYQYHDILCLAGIILRLPD 496

Query: 180 DTKTYQAEKARGQQASGIACYMKNPFGATEEDAIAKHICRVVDRALKEASFEYFKPSNDIP 239
 D T E ARG I CYMK+ A+EE+A++H+ ++ A K+ + P
 Sbjct: 497 DLGTSYFELARGDVPKTIQCYMKET-NASEEEAVEHVKFLIREAWKDMN-TAIAAGYPFP 554

Query: 240 MGCKSFIFNLRLCVQIFYKFIDGYGIANEE 269
 G + N+ Q Y DG+G+ + +
 Sbjct: 555 DGMVAGAANIGRVAQFIYLGHDGFGVQHSK 584

TABLE 14

Score = 120 bits (299), Expect = 6e-27
 Identities = 70/272 (25%), Positives = 137/272 (49%), Gaps = 3/272 (1%)

Query: 2 RVVECYFWALGVYFEPQYSQARVMLVKTISMISIVODTFDAYGTVKELEYTDAIQRWDI 61
 R VE Y W + FEP++S++R+ KT + +++DD +D + T+ E++ T+ ++RWD+
 Sbjct: 296 RHVEYYSWVVMCIFEPFSESRIAFKTAILCTVLDDLYDTHATLHEIKIMTEGVRRWDL 355

Query: 62 NEIDRLPDYMKISYKAILDLYKDYEKELSSAGRSHIVCHAIERMKEVVRNYNVESTWFIE 121
 + D LPDY+KI+++ + + E+ + + K + +Y E+ W
 Sbjct: 356 SLTDDLDPYIKIAFQFFFTVNELIVEIVKRQGRDMTTIVKDCWKRYIESYLQEAEWIAT 415

Query: 122 GYMPPVSEYLSNALATTTYYLATTSYLGM-KSATEQDFEWLSKNPKILEASVIICRVID 180
 G++P +EY+ N +A++ L L + K + E + KIL+ + R+ D
 Sbjct: 416 GHIPTFNEYIKNGMASSGMCILNPLNPLLLDKLLPDNILEQIHSPSKILDLELTGRIAD 475

Query: 181 DTATYEVEKSRGQIATGIECCMRDYGISTKE-AMAKFQNMAETAWKDINEGLLRPTPVST 239
 D +E EK RG++A+ ++C M++ ST E A+ + + + ++ N ++ V
 Sbjct: 476 DLKDFEDEKERGEMASSLQCYMKENPESTVENALNHIKGILNRSLEEFNWEFMKQDSVPM 535

Query: 240 EFLTPILNLARIVEVTYIHNLDGYTHPEKVLK 271
 N+ R ++ Y + DG +K +K
 Sbjct: 536 CCKKFTFNIGRGLQFIYKYR-DGLYISDKEVK 566

TABLE 15

Score = 221 bits (557), Expect = 4e-57
 Identities = 120/283 (42%), Positives = 178/283 (62%), Gaps = 6/283 (2%)

Query: 5 EFYFWMAAAISEPEFSGSRVAFTKIAILMTMLDDLYDTHGTL DQLKIFTEGVRRWDVSLV 64
 E YF A+ I EPEFS R +TK + +LDDLYD HG+LD LK+FTE V+RWD+SLV
 Sbjct: 589 EIYFSPASFIFEPEFSKCREVYTKTSNFTVILDDLYDAHGSLDDLKLFTE SVKRWDSL V 648

Query: 65 EGLPDFMKIAFEFWLKTSNELIAEAVKAQQQDMAAYIRKNAWERYLEAYLQDAEWIATGH 124
 + +P MKI F + T N++ E + QG+D+ YI +N W+ LEAY ++AEW +
 Sbjct: 649 DQMPQQMKICFVG FYNTFNDIAKEGRERQGRDVLGYI-QNVWKVQLEAYTKEAEWSEAKY 707

Query: 125 VPTFDEYLNNGTPNTGMCVNLNLIPLLLMGEHLPIDILEQIFLPSRFHHLIELASRLVDDA 184
 VP+F+EY+ N + + + LI L GE L ++L +I SRF L+ L RLV+D
 Sbjct: 708 VPSFNEYIENASVSIALGTVV LISA LFTGEVLTDEVLSKIDRESRFLQLMGLTGRLVNDT 767

Query: 185 RDFQAEKDHGDL-SCIECYLKDHP ESTVEDALNHVNGLLGNCLLEMNWKFLKKQDSVPLS 243
 + +QAE+ G++ S I+CY+KDHP+ + E+AL HV ++ N L E+N +F+ + +P
 Sbjct: 768 KTYQAERGQGEVASAIQCYMKDHPKISEEEALQHVYSVMENALEELNREFV--NNKIPDI 825

Query: 244 CKKYSFHV LARS IQFMYNQGDGFSISNKV-IKDQVQKVLIVPV 285
 K+ F AR +Q Y QGDG ++S+ + IK+ V+ L PV
 Sbjct: 826 YKRLVFET-ARIMQLFYMQGDGLT LSHDMEIKEHVKNCLFQPV 867

WE CLAIM THE FOLLOWING:

1. An isolated terpene synthase having a region with 20% or greater sequence identity to residues 265 to 535 of SEQ ID NO: 2, said synthase comprising nine α -carbons having interatomic distances in Angstroms between said α -carbons that are ± 2.3 Angstroms of the following interatomic distances:

| α -Carbon | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 |
|------------------|------|------|------|------|------|------|------|------|------|
| 1 | 0.0 | 8.4 | 13.7 | 12.7 | 11.9 | 10.2 | 13.1 | 9.4 | 12.8 |
| 2 | 8.4 | 0.0 | 11.3 | 8.7 | 10.2 | 7.2 | 14.8 | 15.1 | 17.4 |
| 3 | 13.7 | 11.3 | 0.0 | 3.8 | 5.4 | 9.3 | 6.6 | 13.9 | 13.7 |
| 4 | 12.7 | 8.7 | 3.8 | 0.0 | 3.8 | 6.0 | 9.2 | 15.4 | 16.1 |
| 5 | 11.9 | 10.2 | 5.4 | 3.8 | 0.0 | 5.0 | 7.8 | 14.6 | 15.5 |
| 6 | 10.2 | 7.2 | 9.3 | 6.0 | 5.0 | 0.0 | 12.0 | 16.1 | 18.0 |
| 7 | 13.1 | 14.8 | 6.6 | 9.2 | 7.8 | 12.0 | 0.0 | 10.2 | 9.5 |
| 8 | 9.4 | 15.1 | 13.9 | 15.4 | 14.6 | 16.1 | 10.2 | 0.0 | 3.8 |
| 9 | 12.8 | 17.4 | 13.7 | 16.1 | 15.5 | 18.0 | 9.5 | 3.8 | 0.0 |

the center point of each said α -carbon positioned within a sphere having a radius of 2.3 Angstroms, the center points of each said sphere having the following structural coordinates:

| α -Carbon Number | X Position | Y Position | Z Position |
|-------------------------|------------|------------|------------|
| 1 | 120.203 | 38.695 | 43.506 |
| 2 | 114.058 | 43.884 | 41.015 |
| 3 | 106.807 | 36.336 | 45.151 |
| 4 | 107.629 | 38.010 | 41.804 |
| 5 | 109.375 | 34.842 | 40.617 |
| 6 | 111.944 | 37.854 | 37.602 |
| 7 | 110.233 | 31.098 | 47.361 |
| 8 | 118.846 | 34.443 | 51.796 |
| 9 | 116.461 | 32.848 | 54.290 |

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, each said α -carbon having an associated R-group, said synthase having an ordered arrangement of said R-groups other than the following ordered arrangements of R-groups:

Table 9

| Ordered Arrangements of α -Carbons 1-9 | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 |
| A | W | I | T | T | Y | L | C | T | Y |
| B | W | I | S | T | Y | L | C | T | Y |
| C | W | I | C | G | Y | L | C | T | Y |
| D | W | I | S | G | Y | L | C | T | Y |
| E | W | L | A | G | Y | L | A | V | Y |
| F | W | L | T | V | H | L | G | L | Y |
| G | W | L | A | G | Y | L | A | V | Y |
| H | W | I | V | G | N | L | F | S | Y |
| I | W | I | T | A | G | L | S | T | Y |
| J | W | V | S | C | I | M | G | M | Y |
| K | F | F | I | T | A | T | G | L | Y |
| L | W | N | I | S | G | M | L | S | Y |
| M | W | V | S | S | Y | L | G | M | Y |
| N | F | F | T | L | A | L | G | L | Y |
| O | W | N | S | G | P | L | L | M | Y |
| P | W | N | G | G | I | L | L | I | Y |
| Q | Y | L | V | T | M | T | G | I | Y |
| R | W | I | I | S | A | I | L | I | Y |
| S | W | F | S | S | V | I | L | I | Y |
| T | W | I | V | A | S | I | L | I | Y |
| U | W | N | I | S | S | I | F | M | Y |
| V | L | A | I | G | Q | L | S | I | F |
| W | S | S | I | A | L | V | G | F | Y |
| X | L | C | C | G | H | S | L | Y | Y |
| Y | S | F | S | S | V | I | L | Y | Y |
| Z | W | A | S | G | M | L | G | V | Y |

Table 9

| | | | | | | | | | | | | | |
|----|---|---|---|---|---|---|---|---|---|---|---|---|---|
| AA | A | N | L | T | S | T | C | L | Y | T | C | L | Y |
| BB | L | C | S | A | Y | V | L | L | Y | V | L | L | Y |
| CC | W | A | T | G | M | L | L | M | M | L | S | M | Y |
| DD | M | C | S | S | G | V | S | G | G | C | L | V | Y |
| EE | S | G | V | G | L | A | G | L | Y | W | F | Y | Y |
| FF | S | G | A | L | G | A | G | L | Y | F | F | Y | Y |
| GG | S | G | F | A | L | F | G | L | Y | F | F | Y | Y |
| HH | A | G | F | A | L | F | G | L | Y | F | F | Y | Y |
| II | W | V | T | G | L | V | L | L | Y | S | I | Y | Y |
| JJ | W | A | S | G | M | L | L | L | Y | S | I | Y | Y |
| KK | W | I | S | T | Y | L | L | L | Y | C | C | Y | Y |
| LL | W | I | T | T | Y | L | L | L | Y | C | C | Y | Y |
| MM | W | N | I | S | G | L | L | L | Y | C | C | Y | Y |
| NN | A | A | I | G | Q | L | L | L | Y | C | C | Y | Y |
| OO | A | I | V | A | S | L | L | L | Y | C | C | Y | Y |

2. The synthase of claim 1, wherein said synthase has 25% or greater sequence identity to residues 265 to 535 of SEQ ID 2.
- 5 3. The synthase of claim 2, wherein said synthase has 35% or greater sequence identity to residues 265 to 535 of SEQ ID 2.
4. The synthase of claim 1, wherein said synthase catalyses the formation of a terpenoid product from a monoterpene substrate.
- 10 5. The synthase of claim 1, wherein said synthase catalyses the formation of a terpenoid product from a sesquiterpene substrate.
6. The synthase of claim 1, wherein said synthase catalyses the formation of a terpenoid product from a diterpene substrate.
- 15 7. The synthase of claims 4, 5, or 6, wherein said product is a cyclic terpenoid hydrocarbon.
- 20 8. The synthase of claim 4, 5, or 6, wherein said product is an acyclic terpenoid hydrocarbon.
9. The synthase of claim 4, 5, or 6 wherein said product is a cyclic hydroxylated terpenoid hydrocarbon.
- 25 10. The synthase of claim 4, 5, or 6 wherein said product is an acyclic hydroxylated terpenoid hydrocarbon.
11. The synthase of claim 1, wherein said R-group associated with said α -carbon 1 is selected from the group consisting of Cys, Ser, and Thr.
- 30 12. The synthase of claim 1, wherein said R-group associated with said α -carbon 1 is selected from the group consisting of Phe, Tyr and Trp.

13. The synthase of claim 1, wherein said R-group associated with said α -carbon 1 is selected from the group consisting of Pro, Gly, and Ala.
14. The synthase of claim 1, wherein said R-group associated with said α -carbon 1 is selected from the group consisting of Glu and Asp.
15. The synthase of claim 1, wherein said R-group associated with said α -carbon 1 is selected from the group consisting of Met, Ile, Val and Leu.
16. The synthase of claim 1, wherein said R-group associated with said α -carbon 1 is selected from the group consisting of Arg and Lys.
17. The synthase of claim 1, wherein said R-group associated with said α -carbon 1 is selected from the group consisting of Gln, Asn and His.
18. The synthase of claim 1, wherein said R-group associated with said α -carbon 2 is selected from the group consisting of Cys, Ser and Thr.
19. The synthase of claim 1, wherein said R-group associated with said α -carbon 2 is selected from the group consisting of Phe, Tyr and Trp.
20. The synthase of claim 1, wherein said R-group associated with said α -carbon 2 is selected from the group consisting of Pro, Gly, and Ala.
21. The synthase of claim 1, wherein said R-group associated with said α -carbon 2 is selected from the group consisting of Glu and Asp.
22. The synthase of claim 1, wherein said R-group associated with said α -carbon 2 is selected from the group consisting of Met, Ile, Val and Leu.
23. The synthase of claim 1, wherein said R-group associated with said α -carbon 2 is selected from the group consisting of Arg and Lys.
24. The synthase of claim 1, wherein said R-group associated with said α -carbon 2 is selected from the group consisting of Gln, Asn and His.

25. The synthase of claim 1, wherein said R-group associated with said α -carbon 3 is selected from the group consisting of Cys, Ser and Thr.
- 5 26. The synthase of claim 1, wherein said R-group associated with said α -carbon 3 is selected from the group consisting of Phe, Tyr and Trp.
27. The synthase of claim 1, wherein said R-group associated with said α -carbon 3 is selected from the group consisting of Pro, Gly, and Ala.
- 10 28. The synthase of claim 1, wherein said R-group associated with said α -carbon 3 is selected from the group consisting of Glu and Asp.
29. The synthase of claim 1, wherein said R-group associated with said α -carbon 3 is selected from the group consisting of Met, Ile, Val and Leu.
- 15 30. The synthase of claim 1, wherein said R-group associated with said α -carbon 3 is selected from the group consisting of Arg and Lys.
31. The synthase of claim 1, wherein said R-group associated with said α -carbon 3 is selected from the group consisting of Gln, Asn and His.
- 20 32. The synthase of claim 1, wherein said R-group associated with said α -carbon 4 is selected from the group consisting of Cys, Ser and Thr.
- 25 33. The synthase of claim 1, wherein said R-group associated with said α -carbon 4 is selected from the group consisting of Phe, Tyr and Trp.
34. The synthase of claim 1, wherein said R-group associated with said α -carbon 4 is selected from the group consisting of Pro, Gly, and Ala.
- 30 35. The synthase of claim 1, wherein said R-group associated with said α -carbon 4 is selected from the group consisting of Glu and Asp.

36. The synthase of claim 1, wherein said R-group associated with said α -carbon 4 is selected from the group consisting of Met, Ile, Val and Leu.
37. The synthase of claim 1, wherein said R-group associated with said α -carbon 4 is selected from the group consisting of Arg and Lys.
38. The synthase of claim 1, wherein said R-group associated with said α -carbon 4 is selected from the group consisting of Gln, Asn and His.
39. The synthase of claim 1, wherein said R-group associated with said α -carbon 5 is selected from the group consisting of Cys, Ser and Thr.
40. The synthase of claim 1, wherein said R-group associated with said α -carbon 5 is selected from the group consisting of Phe, Tyr and Trp.
41. The synthase of claim 1, wherein said R-group associated with said α -carbon 5 is selected from the group consisting of Pro, Gly, and Ala.
42. The synthase of claim 1, wherein said R-group associated with said α -carbon 5 is selected from the group consisting of Glu and Asp.
43. The synthase of claim 1, wherein said R-group associated with said α -carbon 5 is selected from the group consisting of Met, Ile, Val and Leu.
44. The synthase of claim 1, wherein said R-group associated with said α -carbon 5 is selected from the group consisting of Arg and Lys.
45. The synthase of claim 1, wherein said R-group associated with said α -carbon 5 is selected from the group consisting of Gln, Asn and His.
46. The synthase of claim 1, wherein said R-group associated with said α -carbon 6 is selected from the group consisting of Cys, Ser and Thr.
47. The synthase of claim 1, wherein said R-group associated with said α -carbon 6 is selected from the group consisting of Phe, Tyr and Trp.

48. The synthase of claim 1, wherein said R-group associated with said α -carbon 6 is selected from the group consisting of Pro, Gly, and Ala.
- 5 49. The synthase of claim 1, wherein said R-group associated with said α -carbon 6 is selected from the group consisting of Glu and Asp.
50. The synthase of claim 1, wherein said R-group associated with said α -carbon 6 is selected from the group consisting of Met, Ile, Val and Leu.
- 10 51. The synthase of claim 1, wherein said R-group associated with said α -carbon 6 is selected from the group consisting of Arg and Lys.
52. The synthase of claim 1, wherein said R-group associated with said α -carbon 6 is selected from the group consisting of Gln, Asn and His.
- 15 53. The synthase of claim 1, wherein said R-group associated with said α -carbon 7 is selected from the group consisting of Cys, Ser and Thr.
- 20 54. The synthase of claim 1, wherein said R-group associated with said α -carbon 7 is selected from the group consisting of Phe, Tyr and Trp.
55. The synthase of claim 1, wherein said R-group associated with said α -carbon 7 is selected from the group consisting of Pro, Gly, and Ala.
- 25 56. The synthase of claim 1, wherein said R-group associated with said α -carbon 7 is selected from the group consisting of Glu and Asp.
57. The synthase of claim 1, wherein said R-group associated with said α -carbon 7 is selected from the group consisting of Met, Ile, Val and Leu.
- 30 58. The synthase of claim 1, wherein said R-group associated with said α -carbon 7 is selected from the group consisting of Arg and Lys.

59. The synthase of claim 1, wherein said R-group associated with said α -carbon 7 is selected from the group consisting of Gln, Asn and His.
60. The synthase of claim 1, wherein said R-group associated with said α -carbon 8 is selected from the group consisting of Cys, Ser and Thr.
61. The synthase of claim 1, wherein said R-group associated with said α -carbon 8 is selected from the group consisting of Phe, Tyr and Trp.
62. The synthase of claim 1, wherein said R-group associated with said α -carbon 8 is selected from the group consisting of Pro, Gly, and Ala.
63. The synthase of claim 1, wherein said R-group associated with said α -carbon 8 is selected from the group consisting of Glu and Asp.
64. The synthase of claim 1, wherein said R-group associated with said α -carbon 8 is selected from the group consisting of Met, Ile, Val and Leu.
65. The synthase of claim 1, wherein said R-group associated with said α -carbon 8 is selected from the group consisting of Arg and Lys.
66. The synthase of claim 1, wherein said R-group associated with said α -carbon 8 is selected from the group consisting of Gln, Asn and His.
67. The synthase of claim 1, wherein said R-group associated with said α -carbon 9 is selected from the group consisting of Cys, Ser and Thr.
68. The synthase of claim 1, wherein said R-group associated with said α -carbon 9 is selected from the group consisting of Phe, Tyr and Trp.
69. The synthase of claim 1, wherein said R-group associated with said α -carbon 9 is selected from the group consisting of Pro, Gly, and Ala.
70. The synthase of claim 1, wherein said R-group associated with said α -carbon 9 is selected from the group consisting of Glu and Asp.

71. The synthase of claim 1, wherein said R-group associated with said α -carbon 9 is selected from the group consisting of Met, Ile, Val and Leu.
- 5 72. The synthase of claim 1, wherein said R-group associated with said α -carbon 9 is selected from the group consisting of Arg and Lys.
73. The synthase of claim 1, wherein said R-group associated with said α -carbon 9 is selected from the group consisting of Gln, Asn and His.
- 10 74. The synthase of claim 1, wherein said ordered arrangement of R-groups in said synthase associated with said α -carbons 1 to 9 is Trp, Ile, Thr, Thr, Tyr, Leu, Cys, Thr and Phe, respectively.
- 15 75. The synthase of claim 1, wherein said ordered arrangement of R-groups in said synthase associated with said α -carbons 1 to 9 is Ser, Ile, Thr, Thr, Tyr, Leu, Cys, Thr and Tyr, respectively.
- 20 76. The synthase of claim 1, wherein said ordered arrangement of R-groups in said synthase associated with said α -carbons 1 to 9 is Trp, Ile, Thr, Thr, Tyr, Leu, Trp, Thr and Tyr, respectively.
- 25 77. The synthase of claim 1, wherein said ordered arrangement of R-groups in said synthase associated with said α -carbons 1 to 9 is Ser, Ile, Thr, Thr, Tyr, Leu, Trp, Thr and Tyr, respectively.
- 30 78. The synthase of claim 1, wherein said ordered arrangement of R-groups in said synthase associated with said α -carbons 1 to 9 is Glu, Ile, Thr, Thr, Tyr, Leu, Cys, Thr and Tyr, respectively.
- 35 79. A terpene synthase made by aligning a primary amino acid sequence of a terpene synthase polypeptide to the amino acid sequence of residues 265 to 535 of SEQ ID NO: 2, mutating a nucleic acid encoding said polypeptide at one or more codons of nine amino acid residues in a region of said polypeptide having 20% or greater sequence identity to residues 265 to 535 of SEQ ID NO: 2, said nine residues

in said polypeptide aligning with residues 273, 294, 402, 403, 404, 407, 440, 519 and 520 of SEQ ID NO: 2; and expressing said mutated nucleic acid so that a mutated terpene synthase is made.

- 5 80. An isolated terpene synthase having a region with 20% or greater sequence identity to residues 265 to 535 of SEQ ID NO: 2, said synthase comprising sixteen α -carbons, said α -carbons having interatomic distances in Angstroms between said α -carbons that are ± 2.3 Angstroms of the following interatomic distances:

| α -Carbon | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 |
|------------------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| 1 | 0.0 | 5.0 | 6.0 | 10.5 | 9.0 | 14.3 | 13.0 | 13.5 | 11.2 | 15.6 | 12.5 | 11.8 | 15.0 | 13.7 | 8.3 | 11.0 |
| 2 | 5.0 | 0.0 | 8.4 | 13.3 | 12.4 | 13.7 | 12.7 | 11.9 | 10.2 | 13.1 | 9.2 | 9.4 | 12.8 | 13.6 | 9.3 | 12.9 |
| 3 | 6.0 | 8.4 | 0.0 | 5.3 | 6.0 | 11.3 | 8.7 | 10.2 | 7.2 | 14.8 | 13.9 | 15.1 | 17.4 | 15.7 | 11.3 | 13.3 |
| 4 | 10.5 | 13.3 | 5.3 | 0.0 | 3.8 | 10.7 | 8.3 | 11.4 | 9.6 | 16.1 | 16.8 | 18.1 | 19.6 | 16.8 | 13.3 | 13.9 |
| 5 | 9.0 | 12.4 | 6.0 | 3.8 | 0.0 | 10.8 | 9.6 | 12.5 | 11.6 | 15.5 | 15.4 | 15.9 | 17.3 | 13.8 | 10.1 | 10.3 |
| 6 | 14.3 | 13.7 | 11.3 | 10.7 | 10.8 | 0.0 | 3.8 | 5.4 | 9.3 | 6.6 | 10.5 | 13.9 | 13.7 | 12.9 | 12.8 | 14.1 |
| 7 | 13.0 | 12.7 | 8.7 | 8.3 | 9.6 | 3.8 | 0.0 | 3.8 | 6.0 | 9.2 | 12.1 | 15.4 | 16.1 | 15.3 | 13.8 | 15.4 |
| 8 | 13.5 | 11.9 | 10.2 | 11.4 | 12.5 | 5.4 | 3.8 | 0.0 | 5.0 | 7.8 | 10.5 | 14.6 | 15.5 | 16.0 | 14.7 | 17.0 |
| 9 | 11.2 | 10.2 | 7.2 | 9.6 | 11.6 | 9.3 | 6.0 | 5.0 | 0.0 | 12.0 | 12.8 | 16.1 | 18.0 | 18.2 | 15.3 | 17.8 |
| 10 | 15.6 | 13.1 | 14.8 | 16.1 | 15.5 | 6.6 | 9.2 | 7.8 | 12.0 | 0.0 | 5.9 | 10.2 | 9.5 | 11.4 | 12.8 | 14.9 |
| 11 | 12.5 | 9.2 | 13.9 | 16.8 | 15.4 | 10.5 | 12.1 | 10.5 | 12.8 | 5.9 | 0.0 | 5.0 | 6.0 | 9.5 | 9.7 | 12.8 |
| 12 | 11.8 | 9.4 | 15.1 | 18.1 | 15.9 | 13.9 | 15.4 | 14.6 | 16.1 | 12.2 | 5.0 | 0.0 | 3.8 | 7.1 | 7.2 | 10.2 |
| 13 | 15.0 | 12.8 | 17.4 | 19.6 | 17.3 | 13.7 | 16.1 | 15.5 | 18.0 | 9.5 | 6.0 | 3.8 | 0.0 | 5.8 | 8.8 | 10.8 |
| 14 | 13.7 | 13.6 | 15.7 | 16.8 | 13.8 | 12.9 | 15.3 | 16.0 | 18.2 | 11.4 | 9.5 | 7.1 | 5.8 | 0.0 | 5.7 | 5.7 |
| 15 | 8.3 | 9.3 | 11.3 | 13.3 | 10.1 | 12.8 | 13.8 | 14.7 | 15.3 | 12.8 | 9.7 | 7.2 | 8.8 | 5.7 | 0.0 | 3.8 |
| 16 | 11.0 | 12.9 | 13.3 | 13.9 | 10.3 | 14.1 | 15.4 | 17.0 | 17.8 | 14.9 | 12.8 | 10.2 | 10.8 | 5.7 | 3.8 | 0.0 |

the center point of each said α -carbon positioned within a sphere having a radius of 2.3 Angstroms, the center points of each said sphere having the following structural coordinates:

| α -Carbon Number | X Position | Y Position | Z Position |
|-------------------------|------------|------------|------------|
| 1 | 119.144 | 43.487 | 44.133 |
| 2 | 120.203 | 38.695 | 43.506 |
| 3 | 114.058 | 43.884 | 41.015 |
| 4 | 109.327 | 46.145 | 41.743 |
| 5 | 110.682 | 46.410 | 45.284 |
| 6 | 106.807 | 36.336 | 45.151 |
| 7 | 107.629 | 38.010 | 41.804 |
| 8 | 109.375 | 34.842 | 40.617 |
| 9 | 111.944 | 37.854 | 37.602 |
| 10 | 110.233 | 31.098 | 47.361 |
| 11 | 115.915 | 32.218 | 48.369 |
| 12 | 118.846 | 34.443 | 51.796 |
| 13 | 116.461 | 32.848 | 54.290 |
| 14 | 114.100 | 38.006 | 55.620 |
| 15 | 116.617 | 41.285 | 51.702 |
| 16 | 114.855 | 43.486 | 54.238 |

, each said α -carbon having an associated R-group, said synthase having an ordered arrangement of said R-groups other than the following ordered arrangements of R-groups:

Table 8

| Ordered Arrangement of R-Groups at α -carbons 1-16 | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|----|----|----|----|----|----|----|
| | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 |
| A | C | W | I | I | S | T | T | Y | L | C | V | T | T | D | Y | T |
| B | C | W | I | I | S | S | G | Y | L | C | M | L | Y | D | Y | T |
| C | G | W | I | A | S | C | G | Y | L | C | M | L | Y | D | Y | T |
| D | G | W | I | A | S | S | G | Y | L | C | M | L | Y | D | Y | T |
| E | C | W | L | T | S | A | G | H | L | A | A | L | Y | D | Y | T |
| F | G | W | L | T | S | T | V | Y | L | A | A | L | Y | D | Y | T |
| G | C | W | L | T | S | A | G | H | L | A | A | L | Y | D | Y | T |
| H | C | W | L | T | S | T | V | Y | L | A | A | L | Y | D | Y | T |
| I | L | W | I | V | D | T | A | N | L | F | A | C | Y | D | Y | T |
| J | P | W | I | V | D | T | A | N | L | F | A | C | Y | D | Y | T |
| K | A | W | V | C | G | S | C | I | M | G | I | S | Y | D | Y | T |
| L | N | F | N | L | G | I | S | G | L | G | A | M | Y | D | Y | T |
| M | C | W | V | L | T | S | S | Y | L | G | A | M | Y | D | Y | T |
| N | S | W | V | L | T | S | S | Y | L | G | A | M | Y | D | Y | T |
| O | N | F | N | L | G | I | S | G | L | G | A | M | Y | D | Y | T |
| P | C | W | N | V | T | S | G | P | L | L | A | I | Y | D | Y | T |
| Q | C | W | N | V | T | S | G | P | L | L | A | I | Y | D | Y | T |
| R | C | W | N | V | T | S | G | P | L | L | A | I | Y | D | Y | T |
| S | C | W | N | V | T | S | G | P | L | L | A | I | Y | D | Y | T |
| T | C | W | N | V | T | S | G | P | L | L | A | I | Y | D | Y | T |
| U | C | W | N | V | T | S | G | P | L | L | A | I | Y | D | Y | T |
| V | C | W | N | V | T | S | G | P | L | L | A | I | Y | D | Y | T |
| W | C | W | N | V | T | S | G | P | L | L | A | I | Y | D | Y | T |
| X | C | W | N | V | T | S | G | P | L | L | A | I | Y | D | Y | T |
| Y | C | W | N | V | T | S | G | P | L | L | A | I | Y | D | Y | T |
| Z | C | W | N | V | T | S | G | P | L | L | A | I | Y | D | Y | T |

Table 8

| | | | | | | | | | | | | | | | | | | | |
|----|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| AA | A | A | N | L | T | L | T | S | T | C | L | L | Y | Y | Y | Y | Y | Y | N |
| BB | F | L | C | V | T | S | T | Y | V | L | S | L | M | F | F | F | F | F | S |
| CC | F | W | A | M | T | T | T | M | L | I | T | L | V | F | F | F | F | F | T |
| DD | Y | M | C | V | T | S | T | G | C | I | S | L | L | V | F | F | F | F | T |
| EE | V | S | G | Q | V | V | V | L | V | W | V | G | L | V | F | F | F | F | G |
| FF | C | S | G | T | T | A | T | G | V | G | A | G | L | L | V | F | F | G | T |
| GG | C | S | G | T | T | F | T | L | I | G | A | L | L | L | V | F | F | T | T |
| HH | C | A | G | T | T | F | T | L | I | G | A | L | L | L | V | F | F | T | T |
| II | I | W | V | I | S | T | S | L | V | I | G | L | L | L | V | F | F | T | T |
| JJ | Y | W | A | C | T | S | S | M | L | I | G | L | L | L | V | F | F | T | T |
| KK | C | W | I | I | T | S | S | Y | L | L | C | L | L | L | V | F | F | T | T |
| LL | C | W | I | I | S | T | T | Y | L | L | C | L | L | L | V | F | F | T | T |
| MM | C | W | I | I | T | I | I | G | M | L | C | L | L | L | V | F | F | T | T |
| NN | F | A | N | Q | T | I | I | Q | L | M | C | L | L | L | V | F | F | T | T |
| OO | F | A | I | A | T | V | A | S | L | I | S | L | L | L | V | F | F | T | T |

81. The synthase of claim 80, wherein said synthase has 25% or greater sequence identity to residues 265 to 535 of SEQ ID NO: 2.
82. The synthase of claim 81, wherein said synthase has 35% or greater sequence identity to residues 265 to 535 of SEQ ID NO: 2.
83. The synthase of claim 81, wherein said synthase catalyses the formation of a terpenoid product from a monoterpene substrate.
84. The synthase of claim 81, wherein said synthase catalyses the formation of a terpenoid product from a sesquiterpene substrate.
85. The synthase of claim 81, wherein said synthase catalyses the formation of a terpenoid product from a diterpene substrate.
86. The synthase of claims 83, 84, or 85, wherein said product is a cyclic terpenoid hydrocarbon.
87. The synthase of claim 81, wherein said ordered arrangement of R-groups in said synthase associated with said α -carbons 1 to 16 is Cys, Trp, Ile, Ile, Ser, Thr, Thr, Tyr, Leu, Cys, Val, Thr, Tyr, Asp, Phe and Thr, respectively.
88. An isolated terpene synthase having a region with 20% or greater sequence identity to residues 265 to 535 of SEQ ID NO: 2, said synthase comprising nineteen α -carbons having interatomic distances in Angstroms between said α -carbons that are ± 2.3 Angstroms of the following interatomic distances:

Table 2

| α -carbon | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 |
|------------------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| 1 | 0.0 | 5.0 | 6.0 | 10.5 | 9.0 | 19.8 | 16.6 | 14.3 | 13.0 | 13.5 | 11.2 | 15.6 | 16.7 | 12.5 | 11.8 | 15.0 | 13.7 | 8.3 | 11.0 |
| 2 | 5.0 | 0.0 | 8.4 | 13.3 | 12.4 | 21.3 | 16.8 | 13.7 | 12.7 | 11.9 | 10.2 | 14.8 | 15.4 | 9.2 | 9.4 | 12.8 | 13.6 | 9.3 | 12.9 |
| 3 | 6.0 | 8.4 | 0.0 | 5.3 | 6.0 | 15.3 | 12.8 | 11.3 | 8.7 | 10.2 | 7.2 | 13.1 | 18.6 | 13.9 | 15.1 | 17.4 | 15.7 | 11.3 | 13.3 |
| 4 | 10.5 | 13.3 | 5.3 | 0.0 | 3.8 | 11.0 | 10.4 | 10.7 | 8.3 | 11.4 | 9.6 | 16.1 | 17.0 | 16.8 | 18.1 | 19.6 | 16.8 | 13.3 | 13.9 |
| 5 | 9.0 | 12.4 | 6.0 | 3.8 | 0.0 | 11.8 | 11.1 | 10.8 | 9.6 | 12.5 | 11.6 | 15.5 | 15.2 | 15.4 | 15.9 | 17.3 | 13.8 | 10.1 | 10.3 |
| 6 | 19.8 | 21.3 | 15.3 | 11.0 | 11.8 | 0.0 | 6.4 | 9.9 | 10.2 | 13.6 | 15.5 | 16.2 | 15.8 | 20.0 | 22.2 | 21.8 | 18.7 | 18.5 | 18.0 |
| 7 | 16.6 | 16.8 | 12.6 | 10.4 | 11.1 | 6.4 | 0.0 | 3.8 | 5.0 | 7.6 | 11.0 | 10.1 | 11.1 | 14.3 | 17.4 | 17.0 | 15.3 | 15.3 | 15.9 |
| 8 | 14.3 | 13.7 | 11.3 | 10.7 | 10.6 | 9.9 | 3.8 | 0.0 | 3.8 | 5.4 | 9.3 | 6.6 | 8.6 | 10.5 | 13.9 | 13.7 | 12.9 | 12.8 | 14.1 |
| 9 | 13.0 | 12.7 | 8.7 | 8.3 | 9.6 | 10.2 | 5.0 | 3.8 | 0.0 | 3.8 | 6.0 | 9.2 | 12.1 | 12.1 | 15.4 | 16.1 | 15.3 | 13.8 | 15.4 |
| 10 | 13.5 | 11.9 | 10.2 | 11.4 | 12.5 | 13.6 | 7.6 | 5.4 | 3.8 | 0.0 | 5.0 | 7.8 | 12.4 | 10.5 | 14.6 | 15.5 | 16.0 | 14.7 | 17.0 |
| 11 | 11.2 | 10.2 | 7.2 | 9.8 | 11.6 | 15.5 | 11.0 | 9.3 | 6.0 | 5.0 | 0.0 | 12.0 | 16.2 | 12.8 | 16.1 | 18.0 | 18.2 | 15.3 | 17.8 |
| 12 | 15.6 | 13.1 | 14.8 | 16.1 | 15.5 | 16.2 | 10.1 | 6.6 | 9.2 | 7.8 | 12.0 | 0.0 | 6.0 | 5.9 | 10.2 | 9.5 | 11.4 | 12.8 | 14.9 |
| 13 | 16.7 | 15.4 | 16.6 | 17.0 | 15.2 | 15.8 | 11.1 | 8.6 | 12.1 | 12.4 | 16.2 | 6.0 | 0.0 | 8.2 | 9.8 | 7.4 | 7.3 | 11.0 | 11.7 |
| 14 | 12.5 | 8.2 | 13.9 | 16.8 | 15.4 | 20.0 | 14.3 | 10.5 | 12.1 | 10.5 | 12.8 | 5.9 | 8.2 | 0.0 | 5.0 | 6.0 | 9.5 | 9.7 | 12.8 |
| 15 | 11.8 | 9.4 | 15.1 | 18.1 | 15.9 | 22.2 | 17.4 | 13.9 | 15.4 | 14.6 | 16.1 | 10.2 | 9.8 | 5.0 | 0.0 | 3.8 | 7.1 | 7.2 | 10.2 |
| 16 | 15.0 | 12.8 | 17.4 | 19.6 | 17.3 | 21.8 | 17.0 | 13.7 | 16.1 | 15.5 | 18.0 | 9.5 | 7.4 | 6.0 | 3.8 | 0.0 | 5.8 | 8.8 | 10.8 |
| 17 | 13.7 | 13.6 | 15.7 | 16.8 | 13.8 | 18.7 | 15.3 | 12.9 | 15.3 | 16.0 | 18.2 | 11.4 | 7.3 | 9.5 | 7.1 | 5.8 | 0.0 | 5.7 | 5.7 |
| 18 | 8.3 | 9.3 | 11.3 | 13.3 | 10.1 | 18.5 | 15.3 | 12.8 | 13.8 | 14.7 | 15.3 | 12.8 | 11.0 | 9.7 | 7.2 | 8.8 | 5.7 | 0.0 | 3.8 |
| 19 | 11.0 | 12.9 | 13.3 | 13.9 | 10.3 | 18.0 | 15.9 | 14.1 | 15.4 | 17.0 | 17.8 | 14.9 | 11.7 | 12.8 | 10.2 | 10.8 | 5.7 | 3.8 | 0.0 |

the center point of each said α -carbon positioned within a sphere having a radius of 2.3 Angstroms, the center points of each said sphere having the following structural coordinates:

| α -Carbon Number | X Position | Y Position | Z Position |
|-------------------------|------------|------------|------------|
| 1 | 119.144 | 43.487 | 44.133 |
| 2 | 120.203 | 38.695 | 43.506 |
| 3 | 114.058 | 43.884 | 41.015 |
| 4 | 109.327 | 46.145 | 41.743 |
| 5 | 110.682 | 46.410 | 45.284 |
| 6 | 99.381 | 42.920 | 45.148 |
| 7 | 103.445 | 38.054 | 44.605 |
| 8 | 106.807 | 36.336 | 45.151 |
| 9 | 107.629 | 38.010 | 41.804 |
| 10 | 109.375 | 34.842 | 40.617 |
| 11 | 111.944 | 37.854 | 37.602 |
| 12 | 110.233 | 31.098 | 47.361 |
| 13 | 109.178 | 33.314 | 52.875 |
| 14 | 115.915 | 32.218 | 48.369 |
| 15 | 118.846 | 34.443 | 51.796 |
| 16 | 116.461 | 32.848 | 54.290 |
| 17 | 114.100 | 38.006 | 55.620 |
| 18 | 116.617 | 41.285 | 51.702 |
| 19 | 114.855 | 43.486 | 54.238 |

, each said α -carbon having an associated R-group, said synthase having an ordered arrangement of said R-groups other than the following ordered arrangements of R-groups:

Table 7

| Ordered Arrangement of R-Groups at α -carbons 1-19 | | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|----|----|----|----|----|----|----|----|----|----|
| | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 |
| A | C | W | I | I | S | Y | T | T | T | Y | L | C | D | V | T | Y | D | Y | T |
| B | C | W | I | I | S | Y | T | S | G | Y | L | C | D | I | T | Y | D | Y | T |
| C | G | W | I | A | S | Y | T | C | G | Y | L | C | D | M | L | Y | D | Y | T |
| D | G | W | I | A | S | Y | T | S | G | Y | L | C | D | M | L | Y | D | Y | T |
| E | C | W | L | T | S | Y | S | A | G | Y | L | A | N | A | L | Y | D | Y | T |
| F | C | W | L | T | S | Y | S | A | G | Y | L | A | N | A | L | Y | D | Y | T |
| G | L | W | I | T | T | Y | S | V | G | N | L | A | N | V | L | Y | D | Y | T |
| H | P | W | I | V | D | Y | S | A | G | N | L | A | N | V | L | Y | D | Y | T |
| I | A | W | V | C | G | Y | S | T | A | G | L | S | N | A | L | Y | D | Y | T |
| J | N | F | F | L | G | F | E | S | C | Y | M | G | N | A | L | Y | D | Y | T |
| K | C | W | N | I | T | Y | S | I | T | Y | L | G | N | A | L | Y | D | Y | T |
| L | S | W | V | L | T | Y | S | S | S | Y | L | G | N | A | L | Y | D | Y | T |
| M | N | W | N | L | V | N | S | S | L | A | L | G | N | A | L | Y | D | Y | T |
| N | C | W | F | L | T | Y | S | T | L | P | L | G | N | A | L | Y | D | Y | T |
| O | C | W | N | L | T | Y | S | S | G | I | L | G | N | A | L | Y | D | Y | T |
| P | C | W | N | L | T | Y | S | S | G | I | L | G | N | A | L | Y | D | Y | T |
| Q | C | W | N | L | T | Y | S | S | G | I | L | G | N | A | L | Y | D | Y | T |
| R | C | W | N | L | T | Y | S | S | G | I | L | G | N | A | L | Y | D | Y | T |
| S | S | W | F | I | V | F | S | S | A | V | I | L | N | A | L | Y | D | Y | T |
| T | S | W | F | I | V | F | S | S | A | V | I | L | N | A | L | Y | D | Y | T |
| U | N | W | N | A | T | Y | S | S | A | V | I | L | N | A | L | Y | D | Y | T |
| V | F | W | A | Q | T | Y | S | S | A | V | I | L | N | A | L | Y | D | Y | T |
| W | I | L | S | T | V | Y | S | S | A | V | I | L | N | A | L | Y | D | Y | T |
| X | Y | L | S | T | V | Y | S | S | A | V | I | L | N | A | L | Y | D | Y | T |
| Y | G | S | C | I | T | Y | S | S | A | V | I | L | N | A | L | Y | D | Y | T |
| Z | Y | W | A | C | T | Y | S | S | A | V | I | L | N | A | L | Y | D | Y | T |

Table 7

| | | | | | | | | | | | | | | | | | | | | |
|----|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| AA | A | A | N | L | T | N | A | L | T | S | T | C | M | G | D | M | L | L | N | S |
| BB | F | L | C | V | T | Y | S | S | A | Y | A | S | M | L | G | G | L | L | S | S |
| CC | F | W | A | M | T | Y | N | T | G | M | G | A | G | L | G | N | M | V | T | T |
| DD | Y | M | C | V | T | F | V | S | S | G | S | V | G | L | L | N | F | F | G | T |
| EE | V | S | G | Q | V | Y | S | A | G | L | F | A | L | L | N | N | F | F | T | G |
| FF | C | S | G | T | T | M | F | A | L | L | S | A | L | L | N | N | F | F | T | T |
| GG | C | S | G | T | T | M | S | F | A | L | S | A | L | L | N | N | F | F | T | T |
| HH | C | A | G | T | T | M | S | F | A | L | S | A | L | L | N | N | F | F | T | T |
| II | I | W | V | I | S | Y | S | T | A | L | S | A | L | L | N | N | F | F | T | T |
| JJ | Y | W | A | C | T | Y | S | T | G | L | S | A | L | L | N | N | F | F | T | T |
| KK | C | W | I | I | S | Y | S | S | G | L | S | A | L | L | N | N | F | F | T | T |
| LL | C | W | I | I | S | Y | S | S | G | L | S | A | L | L | N | N | F | F | T | T |
| MM | C | W | N | I | T | Y | S | S | G | L | S | A | L | L | N | N | F | F | T | T |
| NN | F | A | A | Q | T | Y | S | S | G | L | S | A | L | L | N | N | F | F | T | T |
| OO | F | A | I | A | T | Y | S | S | G | L | S | A | L | L | N | N | F | F | T | T |

89. The synthase of claim 88, wherein said synthase has 25% or greater sequence identity to residues 265 to 535 of SEQ ID NO: 2.
90. The synthase of claim 88, wherein said synthase has 35% or greater sequence identity to residues 265 to 535 of SEQ ID NO: 2.
91. The synthase of claim 88, wherein said synthase catalyses the formation of a terpenoid product from a monoterpene substrate.
92. The synthase of claim 88, wherein said synthase catalyses the formation of a terpenoid product from a sesquiterpene substrate.
93. The synthase of claim 88, wherein said synthase catalyses the formation of a terpenoid product from a diterpene substrate.
94. The synthase of claims 91, 92, or 93, wherein said product is a cyclic terpenoid hydrocarbon.
95. A isolated protein comprising:
a first domain having an amino terminal end and a carboxyl terminal end;
said first domain comprising amino acids that align structurally in three-dimensional space with a glycosyl hydrolase catalytic core, said glycosyl hydrolase catalytic core selected from the group consisting of amino acids 36 to 230 of glucoamylase PDB code 3GLY of *Aspergillus awamori* and amino acids 36 to 230 of endoglucanase CelD PDB code 1CLC;
a second domain having an amino terminal end and carboxyl terminal end, said second domain comprising amino acids that align structurally in three-dimensional space with avian FPP synthase, said carboxyl terminal end of said first domain linked to said amino terminal end of said second domain; wherein a region of said second domain has 20% or greater sequence identity to residues 265 to 535 of SEQ ID NO: 2, and wherein said second domain comprises nine α -carbons having interatomic distances in Angstroms between said α -carbons that are ± 2.3 Angstroms of the following interatomic distances:

| α -Carbon | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 |
|------------------|------|------|------|------|------|------|------|------|------|
| 1 | 0.0 | 8.4 | 13.7 | 12.7 | 11.9 | 10.2 | 13.1 | 9.4 | 12.8 |
| 2 | 8.4 | 0.0 | 11.3 | 8.7 | 10.2 | 7.2 | 14.8 | 15.1 | 17.4 |
| 3 | 13.7 | 11.3 | 0.0 | 3.8 | 5.4 | 9.3 | 6.6 | 13.9 | 13.7 |
| 4 | 12.7 | 8.7 | 3.8 | 0.0 | 3.8 | 6.0 | 9.2 | 15.4 | 16.1 |
| 5 | 11.9 | 10.2 | 5.4 | 3.8 | 0.0 | 5.0 | 7.8 | 14.6 | 15.5 |
| 6 | 10.2 | 7.2 | 9.3 | 6.0 | 5.0 | 0.0 | 12.0 | 16.1 | 18.0 |
| 7 | 13.1 | 14.8 | 6.6 | 9.2 | 7.8 | 12.0 | 0.0 | 10.2 | 9.5 |
| 8 | 9.4 | 15.1 | 13.9 | 15.4 | 14.6 | 16.1 | 10.2 | 0.0 | 3.8 |
| 9 | 12.8 | 17.4 | 13.7 | 16.1 | 15.5 | 18.0 | 9.5 | 3.8 | 0.0 |

the center point of each said α -carbon positioned within a sphere having a radius of 2.3 Angstroms, the center point of each said sphere having the following structural coordinates:

| α -Carbon Number | X Position | Y Position | Z Position |
|-------------------------|------------|------------|------------|
| 1 | 120.203 | 38.695 | 43.506 |
| 2 | 114.058 | 43.884 | 41.015 |
| 3 | 106.807 | 36.336 | 45.151 |
| 4 | 107.629 | 38.010 | 41.804 |
| 5 | 109.375 | 34.842 | 40.617 |
| 6 | 111.944 | 37.854 | 37.602 |
| 7 | 110.233 | 31.098 | 47.361 |
| 8 | 118.846 | 34.443 | 51.796 |
| 9 | 116.461 | 32.848 | 54.290 |

, each said α -carbon having an associated R-group, said synthase having an ordered arrangement of R-groups other than the following ordered arrangements of R-groups:

Table 9

| Ordered Arrangements of α -Carbons 1-9 | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 |
| A | W | I | T | T | Y | L | C | T | Y |
| B | W | I | S | T | Y | L | C | T | Y |
| C | W | I | C | G | Y | L | C | T | Y |
| D | W | I | S | G | Y | L | C | T | Y |
| E | W | L | A | G | Y | L | C | T | Y |
| F | W | L | T | V | H | L | C | T | Y |
| G | W | L | A | G | Y | L | C | T | Y |
| H | W | L | V | G | Y | L | C | T | Y |
| I | W | L | T | G | Y | L | C | T | Y |
| J | W | L | S | A | Y | L | C | T | Y |
| K | F | V | I | C | I | L | C | T | Y |
| L | W | N | I | T | A | L | C | T | Y |
| M | W | V | S | S | Y | L | C | T | Y |
| N | F | F | T | S | A | L | C | T | Y |
| O | W | N | S | G | P | L | C | T | Y |
| P | W | N | G | G | I | L | C | T | Y |
| Q | Y | L | V | T | M | L | C | T | Y |
| R | W | I | I | S | A | L | C | T | Y |
| S | W | F | S | S | V | L | C | T | Y |
| T | W | I | V | A | S | L | C | T | Y |
| U | W | N | I | S | S | L | C | T | Y |
| V | L | A | I | G | Q | L | C | T | Y |
| W | S | C | I | A | L | V | C | T | Y |
| X | L | F | C | G | H | S | C | T | Y |
| Y | S | F | S | S | V | I | C | T | Y |
| Z | W | A | S | G | M | L | C | T | Y |

Table 9

| | | | | | | | | | | | |
|----|---|---|---|---|---|---|---|---|---|---|---|
| AA | A | N | L | T | S | T | V | C | Y | L | Y |
| BB | L | C | S | A | Y | A | V | L | M | L | Y |
| CC | W | A | T | G | M | G | L | S | V | M | Y |
| DD | M | C | S | S | G | L | I | L | F | F | Y |
| EE | S | G | V | G | L | G | C | W | F | F | Y |
| FF | S | G | A | L | G | V | V | G | F | F | Y |
| GG | S | G | F | A | L | I | I | G | F | F | Y |
| HH | A | G | F | A | L | I | V | G | S | I | Y |
| II | W | V | T | G | L | L | L | I | T | T | Y |
| JJ | W | A | S | G | M | L | L | G | M | M | Y |
| KK | W | I | S | T | Y | Y | L | C | C | L | Y |
| LL | W | I | T | T | Y | Y | L | C | C | L | Y |
| MM | W | N | I | S | G | Q | M | L | S | I | Y |
| NN | A | A | I | G | Q | S | L | S | I | I | Y |
| OO | A | I | V | A | S | S | I | L | I | I | Y |

96. The protein of claim 95, wherein said synthase has 25% or greater sequence identity to SEQ ID NO: 2.
97. The protein of claim 96, wherein said synthase has 35% or greater sequence identity to SEQ ID NO: 2.
98. The synthase of claim 95, wherein said synthase catalyses the formation of a terpenoid product from a monoterpene substrate.
99. The synthase of claim 95, wherein said synthase catalyses the formation of a terpenoid product from a sesquiterpene substrate.
100. The synthase of claim 95, wherein said synthase catalyses the formation of a terpenoid product from a diterpene substrate.
101. The synthase of claims 98, 99, or 100, wherein said product is a cyclic terpenoid hydrocarbon.
102. An isolated synthase having a region with 40% or greater sequence identity to residues 343 to 612 of SEQ ID NO: 20, wherein one or more amino acid residues of said synthase that align with amino acids at positions 348, 351, 372, 375, 376, 454, 479, 480, 481, 482, 485, 519, 523, 597, 600, 601, 605, 607 and 608 of SEQ ID NO: 20 are residues other than the following ordered arrangements of residues:

claim 102

[illegible]

103. An isolated synthase having a region with 40% or greater sequence identity to residues 316 to 586 of SEQ ID NO: 22, wherein one or more amino acid residues of said synthase that align with amino acids at positions 321, 324, 345, 348, 349, 427, 452, 453, 454, 455, 458, 492, 496, 569, 572, 573, 577, 579 and 580 of SEQ ID NO: 22 are residues other than the following ordered arrangements of residues:

| Ordered Arrangement of Residues | | | | | | | | | | | | | | | | | | | |
|---------------------------------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| | 321 | 324 | 345 | 348 | 349 | 427 | 452 | 453 | 454 | 455 | 458 | 492 | 496 | 569 | 572 | 573 | 577 | 579 | 580 |
| A | C | W | I | I | S | Y | T | T | Y | L | C | D | O | V | T | Y | D | Y | T |
| B | C | W | I | I | S | Y | T | S | T | Y | L | C | D | I | T | Y | D | Y | T |
| C | G | W | I | A | S | Y | T | C | G | Y | L | C | D | M | L | Y | D | Y | T |
| D | G | W | I | A | S | Y | T | S | G | Y | L | C | D | M | L | Y | D | Y | T |
| E | C | W | L | T | S | Y | S | A | G | Y | L | A | N | A | L | Y | D | Y | T |
| F | G | W | L | T | S | Y | S | T | V | H | L | G | D | A | V | Y | D | Y | T |
| G | C | W | L | T | S | Y | S | A | G | Y | L | A | N | A | L | Y | D | Y | T |
| H | L | W | I | T | T | Y | S | V | G | N | L | F | D | V | L | Y | D | F | T |
| I | P | W | I | V | D | Y | S | T | A | G | L | S | D | A | C | Y | D | Y | T |
| J | A | W | V | C | G | F | T | S | C | I | M | G | N | C | S | Y | D | Y | S |
| K | N | F | F | L | G | A | E | I | T | A | T | G | N | I | T | Y | E | F | T |
| L | C | W | N | I | T | Y | S | I | S | A | M | L | D | A | M | Y | D | H | Q |
| M | S | W | V | L | T | Y | S | S | S | Y | L | G | G | V | L | Y | D | F | T |
| N | N | F | F | L | V | N | A | T | S | A | L | L | G | N | L | S | Y | E | T |
| O | C | W | N | I | T | Y | I | S | G | P | L | L | L | D | A | M | Y | D | G |
| P | C | W | N | V | T | Y | I | G | G | I | L | L | D | A | I | Y | D | F | G |
| Q | C | Y | L | L | T | F | A | V | T | M | T | L | G | N | A | T | Y | D | G |
| R | C | W | I | I | T | Y | S | I | S | A | I | L | D | N | I | Y | D | O | G |
| S | S | W | F | I | V | F | S | S | S | V | I | L | N | A | V | I | Y | D | G |
| T | S | W | I | A | T | Y | S | V | A | S | I | L | D | N | I | Y | D | F | G |
| U | N | W | N | L | T | Y | S | I | S | S | I | F | N | S | M | Y | D | H | G |
| V | F | L | A | Q | T | Y | S | I | G | Q | L | S | D | T | I | F | D | F | G |
| W | I | S | S | T | V | Y | S | I | A | L | V | S | N | M | F | Y | D | L | T |
| X | Y | L | C | I | T | Y | S | C | G | H | S | L | L | G | F | G | Y | D | S |
| Y | G | S | F | I | T | F | S | S | S | V | I | L | N | A | V | Y | D | L | S |
| Z | Y | W | A | C | T | Y | S | S | G | M | L | G | N | A | L | Y | D | H | Y |
| AA | A | A | N | L | T | N | A | L | T | S | T | C | M | L | L | Y | D | L | S |
| BB | F | L | C | V | T | Y | S | S | A | Y | V | L | S | G | L | Y | D | F | S |
| CC | F | W | A | V | T | Y | N | T | G | M | L | S | D | D | M | Y | D | Y | T |
| DD | Y | M | C | M | T | F | V | S | S | G | L | S | L | G | N | Y | D | Y | G |
| EE | V | S | G | Q | V | Y | S | V | G | L | C | V | G | N | N | Y | D | Y | T |
| FF | C | S | G | T | T | M | S | F | A | L | G | V | G | N | F | Y | D | F | T |
| GG | C | S | G | T | T | M | S | F | A | A | L | I | G | N | N | Y | D | F | T |
| HH | C | A | G | T | T | M | S | F | A | A | L | I | G | N | N | Y | D | Y | T |
| I | I | W | V | I | S | Y | T | T | G | L | V | I | G | N | N | Y | D | Y | T |
| JJ | Y | W | A | C | T | Y | S | S | G | M | L | G | N | D | S | Y | D | L | T |
| KK | C | W | I | I | S | Y | T | S | T | Y | L | C | D | D | V | Y | D | Y | T |
| LL | C | W | I | I | S | Y | T | T | T | Y | L | C | D | D | I | Y | D | Y | T |
| MM | C | W | A | I | T | Y | S | I | S | G | M | L | S | D | I | M | Y | D | G |
| NN | F | A | A | Q | T | Y | S | I | G | Q | L | S | D | I | I | Y | D | H | G |
| OO | F | A | I | A | T | Y | S | V | A | S | I | L | D | A | I | F | D | F | G |

104. An isolated synthase having a region with 40% or greater sequence identity to residues 352 to 622 of SEQ ID NO: 58, wherein one or more amino acid residues of said synthase that align with amino acids at positions 357, 360, 381, 384, 385, 463, 487, 488, 489, 490, 493, 528, 532, 606, 609, 610, 614, 616 and 617 of SEQ ID NO: 58 are residues other than the following ordered arrangements of residues:

| | Ordered Arrangement of Residues | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|---------------------------------|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 357 | C | C | G | G | C | G | C | L | P | A | N | C | S | N | C | C | C | C | S | S | N | F | I | Y | G | Y | A |
| 360 | W | W | W | W | W | W | W | W | W | F | W | W | W | W | W | W | W | W | W | W | L | S | L | S | W | A | L |
| 381 | I | I | I | I | A | L | L | L | I | V | F | N | V | F | N | A | S | C | F | A | N | C | A | N | C | A | L |
| 384 | I | I | A | S | A | S | T | T | D | G | G | I | T | V | T | T | T | V | T | T | T | T | T | T | T | T | T |
| 385 | S | S | S | S | S | S | S | S | S | F | A | Y | Y | N | Y | Y | F | Y | F | Y | Y | N | Y | Y | F | Y | |
| 463 | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | |
| 487 | T | T | T | T | S | S | S | S | T | E | S | S | S | S | S | S | S | S | S | S | S | S | S | S | S | S | |
| 488 | T | T | S | C | S | A | T | S | A | V | T | S | I | S | S | T | S | G | V | I | S | S | V | I | S | S | |
| 489 | T | T | G | G | G | V | G | G | A | C | T | S | S | L | G | G | T | S | A | S | S | A | S | G | A | G | |
| 490 | Y | Y | Y | Y | Y | H | Y | N | G | T | A | G | Y | A | P | I | M | A | V | S | S | Q | L | H | V | M | |
| 493 | L | L | L | L | L | I | A | G | L | L | M | L | L | L | L | L | L | L | V | S | I | L | T | V | V | L | |
| 528 | C | C | C | C | I | A | G | A | F | S | G | L | G | L | L | L | L | L | F | S | G | L | L | G | C | L | |
| 532 | D | D | D | D | N | D | N | D | N | D | G | N | D | D | N | D | N | D | N | D | N | D | N | D | N | D | |
| 606 | V | I | M | M | A | A | A | V | A | C | I | A | V | L | A | A | I | A | V | A | S | T | M | F | A | L | |
| 610 | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | F | Y | Y | Y | Y | Y | Y | Y | |
| 614 | D | D | D | D | D | D | D | D | D | D | D | D | D | D | D | D | D | D | D | D | D | D | D | D | D | D | |
| 616 | Y | Y | Y | Y | Y | F | Y | Y | F | H | F | F | H | F | F | Y | D | H | F | H | F | L | Y | H | L | Y | |
| 617 | T | T | T | T | T | S | T | T | S | T | O | T | T | G | T | G | G | G | G | T | S | G | Y | N | S | S | |

105. An isolated synthase having a region with 40% or greater sequence identity to amino acid residues 272 to 540 encoded by SEQ ID NO: 33, wherein one or more amino acid residues of said synthase that align with amino acids at positions 277, 280, 301, 304, 305, 383, 408, 409, 410, 411, 414, 448, 452, 524, 527, 528, 532, 534 and 535 encoded by SEQ ID NO: 33 are residues other than the following ordered arrangements of residues:

claim 105

| Ordered Arrangement of Residues | | | | | | | | | | | | | | | |
|---------------------------------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| 277 | 280 | 301 | 304 | 305 | 383 | 408 | 409 | 410 | 414 | 448 | 452 | 524 | 527 | 532 | 534 |
| A | C | C | G | G | C | C | L | P | A | N | S | N | C | C | C |
| B | C | G | G | C | C | L | P | A | N | S | N | C | C | C | C |
| C | W | W | W | W | W | W | W | W | W | W | W | W | W | W | W |
| D | W | W | W | W | W | W | W | W | W | W | W | W | W | W | W |
| E | W | W | W | W | W | W | W | W | W | W | W | W | W | W | W |
| F | W | W | W | W | W | W | W | W | W | W | W | W | W | W | W |
| G | W | W | W | W | W | W | W | W | W | W | W | W | W | W | W |
| H | W | W | W | W | W | W | W | W | W | W | W | W | W | W | W |
| I | W | W | W | W | W | W | W | W | W | W | W | W | W | W | W |
| J | W | W | W | W | W | W | W | W | W | W | W | W | W | W | W |
| K | W | W | W | W | W | W | W | W | W | W | W | W | W | W | W |
| L | W | W | W | W | W | W | W | W | W | W | W | W | W | W | W |
| M | W | W | W | W | W | W | W | W | W | W | W | W | W | W | W |
| N | W | W | W | W | W | W | W | W | W | W | W | W | W | W | W |
| O | W | W | W | W | W | W | W | W | W | W | W | W | W | W | W |
| P | W | W | W | W | W | W | W | W | W | W | W | W | W | W | W |
| Q | W | W | W | W | W | W | W | W | W | W | W | W | W | W | W |
| R | W | W | W | W | W | W | W | W | W | W | W | W | W | W | W |
| S | W | W | W | W | W | W | W | W | W | W | W | W | W | W | W |
| T | W | W | W | W | W | W | W | W | W | W | W | W | W | W | W |
| U | W | W | W | W | W | W | W | W | W | W | W | W | W | W | W |
| V | W | W | W | W | W | W | W | W | W | W | W | W | W | W | W |
| W | W | W | W | W | W | W | W | W | W | W | W | W | W | W | W |
| X | W | W | W | W | W | W | W | W | W | W | W | W | W | W | W |
| Y | W | W | W | W | W | W | W | W | W | W | W | W | W | W | W |
| Z | W | W | W | W | W | W | W | W | W | W | W | W | W | W | W |
| AA | W | W | W | W | W | W | W | W | W | W | W | W | W | W | W |
| BB | W | W | W | W | W | W | W | W | W | W | W | W | W | W | W |
| CC | W | W | W | W | W | W | W | W | W | W | W | W | W | W | W |
| DD | W | W | W | W | W | W | W | W | W | W | W | W | W | W | W |
| EE | W | W | W | W | W | W | W | W | W | W | W | W | W | W | W |
| FF | W | W | W | W | W | W | W | W | W | W | W | W | W | W | W |
| GG | W | W | W | W | W | W | W | W | W | W | W | W | W | W | W |
| HH | W | W | W | W | W | W | W | W | W | W | W | W | W | W | W |
| II | W | W | W | W | W | W | W | W | W | W | W | W | W | W | W |
| JJ | W | W | W | W | W | W | W | W | W | W | W | W | W | W | W |
| KK | W | W | W | W | W | W | W | W | W | W | W | W | W | W | W |
| LL | W | W | W | W | W | W | W | W | W | W | W | W | W | W | W |
| MM | W | W | W | W | W | W | W | W | W | W | W | W | W | W | W |
| NN | W | W | W | W | W | W | W | W | W | W | W | W | W | W | W |
| OO | W | W | W | W | W | W | W | W | W | W | W | W | W | W | W |
| 617 | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T |
| 616 | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y |
| 535 | D | D | D | D | D | D | D | D | D | D | D | D | D | D | D |
| 534 | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y |
| 532 | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T |
| 527 | V | I | M | M | A | A | A | V | A | C | I | A | V | L | A |
| 524 | D | D | D | D | N | D | N | D | N | D | N | D | N | D | N |
| 452 | C | C | C | C | A | G | F | S | G | G | L | G | L | G | L |
| 448 | L | L | L | L | L | L | L | L | L | L | L | L | L | L | L |
| 414 | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y |
| 410 | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T |
| 409 | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T |
| 408 | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T |
| 383 | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y |
| 305 | S | S | S | S | S | S | S | S | S | S | S | S | S | S | S |
| 304 | I | I | I | I | I | I | I | I | I | I | I | I | I | I | I |
| 301 | I | I | I | I | I | I | I | I | I | I | I | I | I | I | I |
| 280 | W | W | W | W | W | W | W | W | W | W | W | W | W | W | W |
| 277 | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C |

106. An isolated synthase having a region with 40% or greater sequence identity to residues 319 to 571 of SEQ ID NO: 42, wherein one or more amino acid residues of said synthase that align with amino acids at positions 324, 327, 348, 351, 352, 430, 455, 456, 457, 458, 461, 495, 499, 571, 574, 575, 579, 581 and 582 of SEQ ID NO: 42 are residues other than the following ordered arrangements of residues:

claim 106

| | | Ordered Arrangement of Residues | | | | | | | | | | | | | | | | | | | |
|----|---|---------------------------------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|--|
| | | 324 | 327 | 348 | 351 | 352 | 430 | 455 | 456 | 457 | 458 | 461 | 495 | 499 | 571 | 574 | 575 | 579 | 581 | 582 | |
| A | C | W | I | I | I | S | Y | T | T | T | Y | L | C | D | V | T | Y | D | Y | T | |
| B | C | W | I | I | I | S | Y | T | S | G | Y | L | C | D | I | L | Y | D | Y | T | |
| C | G | W | I | A | A | S | Y | T | C | G | Y | L | C | D | M | L | Y | D | Y | T | |
| D | G | W | I | A | A | S | Y | T | A | G | Y | L | C | D | A | L | Y | D | Y | T | |
| E | G | W | L | L | T | S | Y | S | A | V | H | L | A | D | A | L | Y | D | Y | T | |
| F | C | W | L | L | T | S | Y | S | A | V | Y | L | A | D | A | L | Y | D | Y | T | |
| G | C | W | L | L | T | S | Y | S | A | V | N | L | A | D | A | L | Y | D | Y | T | |
| H | C | W | L | L | T | S | Y | S | A | V | N | L | A | D | A | L | Y | D | Y | T | |
| I | P | W | L | L | T | S | Y | S | A | V | N | L | A | D | A | L | Y | D | Y | T | |
| J | A | W | L | L | T | S | Y | S | A | V | N | L | A | D | A | L | Y | D | Y | T | |
| K | N | W | L | L | T | S | Y | S | A | V | N | L | A | D | A | L | Y | D | Y | T | |
| L | C | W | L | L | T | S | Y | S | A | V | N | L | A | D | A | L | Y | D | Y | T | |
| M | C | W | L | L | T | S | Y | S | A | V | N | L | A | D | A | L | Y | D | Y | T | |
| N | C | W | L | L | T | S | Y | S | A | V | N | L | A | D | A | L | Y | D | Y | T | |
| O | C | W | L | L | T | S | Y | S | A | V | N | L | A | D | A | L | Y | D | Y | T | |
| P | C | W | L | L | T | S | Y | S | A | V | N | L | A | D | A | L | Y | D | Y | T | |
| Q | C | W | L | L | T | S | Y | S | A | V | N | L | A | D | A | L | Y | D | Y | T | |
| R | C | W | L | L | T | S | Y | S | A | V | N | L | A | D | A | L | Y | D | Y | T | |
| S | C | W | L | L | T | S | Y | S | A | V | N | L | A | D | A | L | Y | D | Y | T | |
| T | C | W | L | L | T | S | Y | S | A | V | N | L | A | D | A | L | Y | D | Y | T | |
| U | C | W | L | L | T | S | Y | S | A | V | N | L | A | D | A | L | Y | D | Y | T | |
| V | C | W | L | L | T | S | Y | S | A | V | N | L | A | D | A | L | Y | D | Y | T | |
| W | C | W | L | L | T | S | Y | S | A | V | N | L | A | D | A | L | Y | D | Y | T | |
| X | C | W | L | L | T | S | Y | S | A | V | N | L | A | D | A | L | Y | D | Y | T | |
| Y | C | W | L | L | T | S | Y | S | A | V | N | L | A | D | A | L | Y | D | Y | T | |
| Z | C | W | L | L | T | S | Y | S | A | V | N | L | A | D | A | L | Y | D | Y | T | |
| AA | C | W | L | L | T | S | Y | S | A | V | N | L | A | D | A | L | Y | D | Y | T | |
| BB | C | W | L | L | T | S | Y | S | A | V | N | L | A | D | A | L | Y | D | Y | T | |
| CC | C | W | L | L | T | S | Y | S | A | V | N | L | A | D | A | L | Y | D | Y | T | |
| DD | C | W | L | L | T | S | Y | S | A | V | N | L | A | D | A | L | Y | D | Y | T | |
| EE | C | W | L | L | T | S | Y | S | A | V | N | L | A | D | A | L | Y | D | Y | T | |
| FF | C | W | L | L | T | S | Y | S | A | V | N | L | A | D | A | L | Y | D | Y | T | |
| GG | C | W | L | L | T | S | Y | S | A | V | N | L | A | D | A | L | Y | D | Y | T | |
| HH | C | W | L | L | T | S | Y | S | A | V | N | L | A | D | A | L | Y | D | Y | T | |
| II | C | W | L | L | T | S | Y | S | A | V | N | L | A | D | A | L | Y | D | Y | T | |
| JJ | C | W | L | L | T | S | Y | S | A | V | N | L | A | D | A | L | Y | D | Y | T | |
| KK | C | W | L | L | T | S | Y | S | A | V | N | L | A | D | A | L | Y | D | Y | T | |
| LL | C | W | L | L | T | S | Y | S | A | V | N | L | A | D | A | L | Y | D | Y | T | |
| MM | C | W | L | L | T | S | Y | S | A | V | N | L | A | D | A | L | Y | D | Y | T | |
| NN | C | W | L | L | T | S | Y | S | A | V | N | L | A | D | A | L | Y | D | Y | T | |
| OO | C | W | L | L | T | S | Y | S | A | V | N | L | A | D | A | L | Y | D | Y | T | |

107. An isolated synthase having a region with 40% or greater sequence identity to residues 579 to 847 of SEQ ID NO: 44, wherein one or more amino acid residues of said synthase that align with amino acids at positions 584, 587, 606, 609, 610, 688, 713, 714, 715, 716, 719, 753, 757, 831, 834, 835, 839, 841 and 842 of SEQ ID NO: 44 are residues other than the following ordered arrangements of residues:

claim 107

| Ordered Arrangement of Residues | | | | | | | | | | | | | | | | | | | |
|---------------------------------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| | 584 | 587 | 606 | 609 | 610 | 688 | 713 | 714 | 715 | 716 | 719 | 753 | 757 | 831 | 834 | 835 | 839 | 841 | 842 |
| A | C | W | I | I | S | Y | T | T | T | Y | L | C | D | V | T | Y | D | Y | T |
| B | C | W | I | I | S | Y | T | S | T | Y | L | C | D | I | T | Y | D | Y | T |
| C | G | W | A | A | S | Y | T | C | G | Y | L | C | D | M | L | Y | D | Y | T |
| D | G | W | A | A | S | Y | T | S | G | Y | L | C | D | A | L | Y | D | Y | T |
| E | G | W | L | T | S | Y | S | A | G | Y | L | C | D | A | V | Y | D | Y | T |
| F | G | W | L | T | S | Y | S | A | G | Y | L | C | D | A | A | Y | D | Y | T |
| G | C | W | L | T | S | Y | S | A | G | Y | L | C | D | A | L | Y | D | Y | T |
| H | C | W | L | T | S | Y | S | A | G | Y | L | C | D | A | V | Y | D | Y | T |
| I | P | W | I | V | D | Y | S | V | A | G | L | S | D | A | C | Y | D | Y | T |
| J | A | W | V | C | G | F | T | S | I | T | M | G | N | I | S | Y | D | Y | T |
| K | N | F | F | L | T | A | E | I | S | G | L | G | N | A | M | Y | D | Y | T |
| L | C | W | N | L | T | Y | S | I | S | Y | L | G | N | V | L | Y | D | Y | T |
| M | S | W | V | L | T | Y | S | T | S | A | L | G | N | L | S | Y | D | Y | T |
| N | N | F | F | L | T | N | A | T | L | A | L | G | N | A | M | Y | D | Y | T |
| O | C | W | N | I | T | Y | I | S | G | P | L | L | D | A | M | Y | D | Y | T |
| P | C | W | N | V | T | Y | I | S | G | P | L | L | D | A | M | Y | D | Y | T |
| Q | C | W | N | V | T | Y | I | S | G | P | L | L | D | A | M | Y | D | Y | T |
| R | C | W | N | V | T | Y | I | S | G | P | L | L | D | A | M | Y | D | Y | T |
| S | S | W | F | I | T | Y | S | S | S | A | L | L | N | A | I | Y | D | Y | T |
| T | S | W | F | I | T | Y | S | S | S | A | L | L | N | A | I | Y | D | Y | T |
| U | N | W | L | A | T | Y | S | S | S | A | L | L | N | A | I | Y | D | Y | T |
| V | F | W | A | Q | T | Y | S | S | S | Q | L | F | N | S | M | Y | D | Y | T |
| W | I | S | A | T | V | Y | S | S | A | L | V | G | N | T | F | Y | D | Y | T |
| X | Y | L | C | I | T | Y | S | S | A | L | V | G | N | T | F | Y | D | Y | T |
| Y | G | L | F | I | T | Y | S | S | A | L | V | G | N | T | F | Y | D | Y | T |
| Z | Y | S | C | I | T | Y | S | S | A | L | V | G | N | T | F | Y | D | Y | T |
| AA | A | W | A | C | T | N | S | S | G | H | S | L | N | F | G | Y | D | Y | T |
| BB | A | L | N | V | T | N | S | S | G | V | S | L | N | F | G | Y | D | Y | T |
| CC | F | W | C | M | T | Y | S | S | G | M | T | L | D | A | L | Y | D | Y | T |
| DD | Y | M | A | V | T | Y | S | S | G | M | T | L | D | A | L | Y | D | Y | T |
| EE | V | S | C | Q | T | Y | S | S | G | M | T | L | D | A | L | Y | D | Y | T |
| FF | C | S | G | G | T | Y | S | S | G | M | T | L | D | A | L | Y | D | Y | T |
| GG | C | S | G | G | T | Y | S | S | G | M | T | L | D | A | L | Y | D | Y | T |
| HH | C | S | G | G | T | Y | S | S | G | M | T | L | D | A | L | Y | D | Y | T |
| II | C | S | G | G | T | Y | S | S | G | M | T | L | D | A | L | Y | D | Y | T |
| JJ | Y | W | V | C | T | Y | S | S | G | M | T | L | D | A | L | Y | D | Y | T |
| KK | C | W | I | I | S | Y | T | S | A | G | L | S | D | A | L | Y | D | Y | T |
| LL | C | W | I | I | S | Y | T | S | A | G | L | S | D | A | L | Y | D | Y | T |
| MM | C | W | I | I | S | Y | T | S | A | G | L | S | D | A | L | Y | D | Y | T |
| NN | F | W | N | A | T | Y | S | S | S | Y | L | G | N | A | L | Y | D | Y | T |
| OO | F | A | I | A | T | Y | S | S | S | Y | L | G | N | A | L | Y | D | Y | T |

108. An isolated synthase having a region with 40% or greater sequence identity to residues 495 to 767 of SEQ ID NO: 46, wherein one or more amino acid residues of said synthase that align with amino acids at positions 500, 503, 524, 527, 528, 606, 631, 632, 633, 634, 637, 674, 678, 751, 754, 755, 759, 761 and 762 of SEQ ID NO: 46 are residues other than the following ordered arrangements of residues:

claim 108

| Ordered Arrangement of Residues | | | | | | | | | | | | | | | |
|---------------------------------|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 500 | C | C | G | G | C | C | L | P | A | N | C | S | N | C | C |
| 503 | W | W | W | W | W | W | W | W | W | W | W | W | W | W | W |
| 504 | I | I | I | I | I | I | I | I | I | I | I | I | I | I | I |
| 507 | I | I | I | I | I | I | I | I | I | I | I | I | I | I | I |
| 510 | L | L | L | L | L | L | L | L | L | L | L | L | L | L | L |
| 513 | L | L | L | L | L | L | L | L | L | L | L | L | L | L | L |
| 516 | L | L | L | L | L | L | L | L | L | L | L | L | L | L | L |
| 519 | L | L | L | L | L | L | L | L | L | L | L | L | L | L | L |
| 522 | L | L | L | L | L | L | L | L | L | L | L | L | L | L | L |
| 525 | L | L | L | L | L | L | L | L | L | L | L | L | L | L | L |
| 528 | S | S | S | S | S | S | S | S | S | S | S | S | S | S | S |
| 531 | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T |
| 532 | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T |
| 533 | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T |
| 534 | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y |
| 537 | L | L | L | L | L | L | L | L | L | L | L | L | L | L | L |
| 540 | L | L | L | L | L | L | L | L | L | L | L | L | L | L | L |
| 543 | L | L | L | L | L | L | L | L | L | L | L | L | L | L | L |
| 546 | L | L | L | L | L | L | L | L | L | L | L | L | L | L | L |
| 549 | L | L | L | L | L | L | L | L | L | L | L | L | L | L | L |
| 552 | L | L | L | L | L | L | L | L | L | L | L | L | L | L | L |
| 555 | L | L | L | L | L | L | L | L | L | L | L | L | L | L | L |
| 558 | L | L | L | L | L | L | L | L | L | L | L | L | L | L | L |
| 561 | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y |
| 564 | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y |
| 567 | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y |
| 570 | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y |
| 573 | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y |
| 576 | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y |
| 579 | D | D | D | D | D | D | D | D | D | D | D | D | D | D | D |
| 582 | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T |
| 585 | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T |
| 588 | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T |
| 591 | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T |
| 594 | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T |
| 597 | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T |
| 600 | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T |
| 603 | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T |
| 606 | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y |
| 609 | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y |
| 612 | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y |
| 615 | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y |
| 618 | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y |
| 621 | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y |
| 624 | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y |
| 627 | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y |
| 630 | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y |
| 633 | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T |
| 636 | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T |
| 639 | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T |
| 642 | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T |
| 645 | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T |
| 648 | D | D | D | D | D | D | D | D | D | D | D | D | D | D | D |
| 651 | V | V | V | V | V | V | V | V | V | V | V | V | V | V | V |
| 654 | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T |
| 657 | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T |
| 660 | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T |
| 663 | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T |
| 666 | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T |
| 669 | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T |
| 672 | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T |
| 675 | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T |
| 678 | D | D | D | D | D | D | D | D | D | D | D | D | D | D | D |
| 681 | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y |
| 684 | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y |
| 687 | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y |
| 690 | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y |
| 693 | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y |
| 696 | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y |
| 699 | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y |
| 702 | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y |
| 705 | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y |
| 708 | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y |
| 711 | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y |
| 714 | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y |
| 717 | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y |
| 720 | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y |
| 723 | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y |
| 726 | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y |
| 729 | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y |
| 732 | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y |
| 735 | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y |
| 738 | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y |
| 741 | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y |
| 744 | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y |
| 747 | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y |
| 750 | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y |
| 753 | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y |
| 756 | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y |
| 759 | D | D | D | D | D | D | D | D | D | D | D | D | D | D | D |
| 762 | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T |

109. An isolated synthase having a region with 40% or greater sequence identity to residues 295 to 564 of SEQ ID NO: 48, wherein one or more amino acid residues of said synthase that align with amino acids at positions 300, 303, 324, 327, 328, 406, 431, 432, 433, 434, 437, 471, 475, 548, 551, 552, 556, 558 and 559 of SEQ ID NO: 48 are residues other than the following ordered arrangements of residues:

| | Ordered Arrangement of Residues | | | | | | | | | | | | | | | | | | | |
|----|---------------------------------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|--|
| A | 300 | 303 | 324 | 327 | 328 | 408 | 431 | 432 | 433 | 434 | 437 | 471 | 475 | 548 | 551 | 552 | 556 | 558 | 559 | |
| B | C | W | I | I | S | Y | T | T | T | Y | L | C | D | V | T | Y | D | Y | T | |
| C | C | W | I | I | S | Y | T | S | G | Y | L | C | D | M | T | Y | D | Y | T | |
| D | G | W | I | A | S | Y | T | S | G | Y | L | C | D | M | L | Y | D | Y | T | |
| E | C | W | L | T | S | Y | S | A | G | Y | L | C | N | A | L | Y | D | Y | T | |
| F | G | W | L | L | S | Y | S | T | V | H | L | A | D | A | V | Y | D | Y | T | |
| G | C | W | L | T | S | Y | S | A | G | Y | L | F | D | V | Y | Y | D | Y | T | |
| H | L | W | I | T | T | Y | S | V | G | N | L | S | D | A | Y | Y | D | Y | T | |
| I | P | W | V | V | D | Y | S | T | A | G | M | G | N | C | Y | Y | D | Y | T | |
| J | A | W | F | C | G | F | T | S | C | I | T | G | N | I | Y | Y | D | Y | T | |
| K | N | W | N | L | G | A | E | I | T | A | M | L | N | A | Y | Y | D | Y | T | |
| L | C | W | I | I | T | Y | S | I | S | G | L | L | D | I | Y | Y | D | Y | T | |
| M | S | W | V | L | G | Y | S | S | L | Y | L | G | G | A | Y | Y | D | Y | T | |
| N | N | W | F | L | T | Y | S | T | G | A | L | G | N | V | L | Y | D | Y | T | |
| O | C | W | N | I | T | Y | I | S | G | P | L | L | D | L | S | Y | D | Y | T | |
| P | C | W | N | V | T | Y | I | S | G | I | L | L | D | A | M | Y | D | Y | T | |
| Q | C | W | N | L | T | Y | A | V | T | M | T | L | N | A | T | Y | D | Y | T | |
| R | C | W | I | I | T | F | S | I | S | A | I | L | N | I | I | Y | D | Y | T | |
| S | S | W | F | I | V | Y | S | S | S | V | I | L | N | A | I | Y | D | Y | T | |
| T | S | W | I | A | T | Y | S | V | A | S | I | L | N | S | M | Y | D | Y | T | |
| U | N | W | N | L | T | Y | S | I | S | Y | I | L | N | S | I | Y | D | Y | T | |
| V | F | W | A | Q | T | Y | S | I | A | P | I | L | N | L | I | Y | D | Y | T | |
| W | N | W | N | I | T | Y | S | I | G | I | I | L | N | A | I | Y | D | Y | T | |
| X | I | S | S | I | T | Y | S | I | A | L | I | L | N | S | I | Y | D | Y | T | |
| Y | Y | L | C | I | T | Y | S | I | G | H | V | L | N | M | F | Y | D | Y | T | |
| Z | G | S | F | I | T | F | S | S | S | V | S | L | N | F | G | Y | D | Y | T | |
| AA | Y | W | A | C | T | Y | S | S | G | M | L | G | N | A | V | Y | D | Y | T | |
| BB | F | L | C | V | T | N | A | T | T | S | V | C | M | L | L | Y | D | Y | T | |
| CC | F | W | A | M | T | Y | N | S | G | M | L | L | D | L | M | Y | D | Y | T | |
| DD | Y | M | C | V | T | F | V | S | S | G | I | L | N | I | V | Y | D | Y | T | |
| EE | V | S | G | Q | V | Y | S | V | G | L | C | W | N | V | F | Y | D | Y | T | |
| FF | C | S | G | T | T | M | F | A | L | G | V | G | N | L | F | Y | D | Y | T | |
| GG | C | S | G | T | T | M | S | F | L | L | C | G | N | L | F | Y | D | Y | T | |
| HH | C | A | G | T | T | M | S | F | A | L | C | G | N | L | F | Y | D | Y | T | |
| II | I | W | V | I | S | Y | T | T | G | L | V | I | D | T | Y | Y | D | Y | T | |
| JJ | Y | W | A | C | T | Y | S | S | G | L | L | G | N | L | I | Y | D | Y | T | |
| KK | C | W | I | I | T | Y | T | S | T | | | | | | | | | | | |

110. An isolated synthase having a region with 40% or greater sequence identity to residues 307 to 578 of SEQ ID NO: 50, wherein one or more amino acid residues of said synthase that align with amino acids at positions 312, 315, 336, 339, 340, 419, 444, 445, 446, 447, 450, 484, 488, 562, 565, 566, 570, 572 and 573 of SEQ ID NO: 50 are residues other than the following ordered arrangements of residues:

claim 110

| Ordered Arrangement of Residues | | | | | | | | | | | | | | | | | | | |
|---------------------------------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| | 312 | 315 | 336 | 339 | 340 | 419 | 444 | 445 | 446 | 447 | 450 | 484 | 488 | 562 | 565 | 566 | 570 | 572 | 573 |
| A | C | W | I | I | S | Y | T | T | T | Y | L | C | D | V | T | Y | D | Y | T |
| B | C | W | I | I | S | Y | T | S | T | Y | L | C | D | I | T | Y | D | Y | T |
| C | G | W | I | A | S | Y | T | C | G | Y | L | C | D | M | L | Y | D | Y | T |
| D | G | W | L | A | S | Y | S | A | G | Y | L | A | N | A | L | Y | D | Y | T |
| E | G | W | L | T | S | Y | S | T | V | H | L | G | D | A | V | Y | D | Y | T |
| F | C | W | L | T | S | Y | S | A | G | Y | L | A | N | A | L | Y | D | Y | T |
| G | C | W | L | T | S | Y | S | V | G | Y | L | A | N | A | L | Y | D | Y | T |
| H | L | W | I | V | D | Y | S | T | G | N | L | F | D | A | C | Y | D | Y | T |
| I | P | W | I | C | G | F | T | S | A | G | L | S | D | A | S | Y | D | Y | T |
| J | A | W | V | L | G | Y | S | T | C | I | M | G | N | I | T | Y | D | Y | T |
| K | N | F | N | L | T | Y | S | I | T | A | T | G | N | A | M | Y | D | Y | T |
| L | C | W | N | L | T | Y | S | I | T | G | L | G | N | A | L | Y | D | Y | T |
| M | S | W | V | L | T | Y | S | T | S | Y | L | L | D | A | L | Y | D | Y | T |
| N | N | W | N | V | T | Y | S | T | S | Y | L | L | D | A | L | Y | D | Y | T |
| O | C | W | N | V | T | Y | S | T | S | Y | L | L | D | A | L | Y | D | Y | T |
| P | C | W | N | V | T | Y | S | T | S | Y | L | L | D | A | L | Y | D | Y | T |
| Q | C | W | N | V | T | Y | S | T | S | Y | L | L | D | A | L | Y | D | Y | T |
| R | C | W | N | V | T | Y | S | T | S | Y | L | L | D | A | L | Y | D | Y | T |
| S | S | W | N | V | T | Y | S | T | S | Y | L | L | D | A | L | Y | D | Y | T |
| T | S | W | N | V | T | Y | S | T | S | Y | L | L | D | A | L | Y | D | Y | T |
| U | N | W | N | V | T | Y | S | T | S | Y | L | L | D | A | L | Y | D | Y | T |
| V | F | W | N | V | T | Y | S | T | S | Y | L | L | D | A | L | Y | D | Y | T |
| W | I | W | N | V | T | Y | S | T | S | Y | L | L | D | A | L | Y | D | Y | T |
| X | I | W | N | V | T | Y | S | T | S | Y | L | L | D | A | L | Y | D | Y | T |
| Y | G | W | N | V | T | Y | S | T | S | Y | L | L | D | A | L | Y | D | Y | T |
| Z | Y | W | N | V | T | Y | S | T | S | Y | L | L | D | A | L | Y | D | Y | T |
| AA | A | W | N | V | T | Y | S | T | S | Y | L | L | D | A | L | Y | D | Y | T |
| BB | F | L | C | M | T | Y | S | T | S | Y | L | L | D | A | L | Y | D | Y | T |
| CC | F | W | A | V | T | Y | S | T | S | Y | L | L | D | A | L | Y | D | Y | T |
| DD | Y | M | A | C | T | Y | S | T | S | Y | L | L | D | A | L | Y | D | Y | T |
| EE | V | S | G | Q | T | Y | S | T | S | Y | L | L | D | A | L | Y | D | Y | T |
| FF | C | S | G | T | T | Y | S | T | S | Y | L | L | D | A | L | Y | D | Y | T |
| GG | C | S | G | T | T | Y | S | T | S | Y | L | L | D | A | L | Y | D | Y | T |
| HH | C | S | G | T | T | Y | S | T | S | Y | L | L | D | A | L | Y | D | Y | T |
| II | T | W | V | C | T | Y | S | T | S | Y | L | L | D | A | L | Y | D | Y | T |
| JJ | Y | W | A | I | S | Y | S | T | S | Y | L | L | D | A | L | Y | D | Y | T |
| KK | C | W | I | I | S | Y | S | T | S | Y | L | L | D | A | L | Y | D | Y | T |
| LL | C | W | I | I | S | Y | S | T | S | Y | L | L | D | A | L | Y | D | Y | T |
| MM | C | W | I | I | S | Y | S | T | S | Y | L | L | D | A | L | Y | D | Y | T |
| NN | F | W | A | I | S | Y | S | T | S | Y | L | L | D | A | L | Y | D | Y | T |
| OO | F | A | T | A | T | Y | S | T | S | Y | L | L | D | A | L | Y | D | Y | T |

111. An isolated synthase having a region with 40% or greater sequence identity to residues 264 to 533 of SEQ ID NO: 52, wherein one or more amino acid residues of said synthase that align with amino acids at positions 269, 272, 293, 296, 297, 375, 401, 402, 403, 404, 407, 441, 445, 517, 520, 521, 525, 527 and 528 of SEQ ID NO: 52 are residues other than the following ordered arrangements of residues:

claim 111

| Ordered Arrangement of Residues | | | | | | | | | | | | | | | |
|---------------------------------|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 269 | A | B | C | D | E | F | G | H | I | J | K | L | M | N | O |
| 272 | W | W | W | W | W | W | W | W | W | W | W | W | W | W | W |
| 293 | I | I | I | I | I | I | I | I | I | I | I | I | I | I | I |
| 296 | I | I | I | I | I | I | I | I | I | I | I | I | I | I | I |
| 297 | S | S | S | S | S | S | S | S | S | S | S | S | S | S | S |
| 375 | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y |
| 401 | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T |
| 402 | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T |
| 403 | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T |
| 404 | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y |
| 407 | L | L | L | L | L | L | L | L | L | L | L | L | L | L | L |
| 441 | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C |
| 445 | D | D | D | D | D | D | D | D | D | D | D | D | D | D | D |
| 517 | V | I | M | A | A | A | A | V | A | C | I | A | V | L | A |
| 520 | T | T | L | L | L | V | L | L | C | S | T | M | L | S | M |
| 521 | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y |
| 525 | D | D | D | D | D | D | D | D | D | D | D | D | D | D | D |
| 527 | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y |
| 528 | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T |

112. An isolated synthase having a region with 40% or greater sequence identity to residues 585 to 853 of SEQ ID NO: 56, wherein one or more amino acid residues of said synthase that align with amino acids at positions 590, 593, 614, 617, 618, 696, 721, 722, 723, 724, 727, 761, 765, 837, 840, 841, 845, 847 and 848 of SEQ ID NO: 56 are residues other than the following ordered arrangements of residues:

claim 112

| Ordered Arrangement of Residues | | | | | | | | | | | | | | | | | | | |
|---------------------------------|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 590 | C | C | G | G | C | G | C | L | P | A | N | C | S | N | C | C | C | C | S |
| 593 | W | W | W | W | W | W | W | W | W | F | N | V | F | N | V | F | N | V | F |
| 614 | I | I | I | I | L | L | L | L | I | V | C | G | L | L | L | L | L | L | I |
| 617 | I | I | I | I | T | L | T | T | T | V | L | T | T | T | T | T | T | T | I |
| 618 | S | S | S | S | S | S | S | S | S | S | S | S | S | S | S | S | S | S | S |
| 696 | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y |
| 721 | T | T | T | T | S | S | S | S | S | S | S | S | S | S | S | S | S | S | S |
| 722 | T | S | T | C | S | A | T | A | V | T | S | I | S | S | S | S | S | S | S |
| 723 | T | T | G | G | G | V | G | G | A | G | A | C | T | S | L | G | T | S | S |
| 724 | Y | Y | Y | Y | Y | H | Y | N | G | I | M | T | A | G | Y | A | P | I | M |
| 727 | L | L | L | L | L | L | L | L | L | L | L | L | L | L | L | L | L | L | L |
| 761 | C | C | C | C | C | A | G | A | F | S | G | L | G | L | G | L | L | L | L |
| 765 | D | D | D | D | D | N | D | N | D | N | D | G | N | D | N | D | N | D | N |
| 837 | V | I | M | M | A | A | A | A | V | A | C | I | A | V | L | A | A | A | I |
| 840 | T | T | L | L | L | V | L | L | C | S | T | M | L | S | M | I | T | I | I |
| 841 | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y |
| 845 | D | D | D | D | D | D | D | D | D | D | D | D | D | D | D | D | D | D | D |
| 847 | Y | Y | Y | Y | Y | Y | Y | Y | F | Y | F | H | F | F | H | F | F | H | F |
| 848 | T | T | T | T | T | S | T | T | S | T | T | T | T | T | T | T | T | T | T |

113. An isolated synthase having a region with 40% or greater sequence identity to residues 307 to 574 of SEQ ID NO: 54, wherein one or more amino acid residues of said synthase that align with amino acids at positions 312, 315, 336, 339, 340, 418, 443, 444, 445, 446, 449, 483, 487, 560, 563, 564, 566, 568 and 569 of SEQ ID NO: 54 are residues other than the following ordered arrangements of residues:

claim 113

| Ordered Arrangement of Residues | | 312 | 315 | 336 | 339 | 340 | 418 | 443 | 444 | 445 | 446 | 449 | 483 | 487 | 560 | 563 | 564 | 566 | 568 | 569 |
|---------------------------------|---|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| A | C | W | I | I | I | S | Y | T | T | T | Y | L | C | D | V | T | Y | D | Y | T |
| B | C | W | I | I | I | S | Y | T | T | T | Y | L | C | D | I | T | Y | D | Y | T |
| C | G | W | I | A | A | S | Y | T | T | T | Y | L | C | D | M | L | Y | D | Y | T |
| D | G | W | L | T | T | S | Y | T | T | T | Y | L | C | D | A | L | Y | D | Y | T |
| E | G | W | L | T | T | S | Y | T | T | T | Y | L | C | D | A | L | Y | D | Y | T |
| F | G | W | L | T | T | S | Y | T | T | T | Y | L | C | D | A | L | Y | D | Y | T |
| G | C | W | L | T | T | S | Y | T | T | T | Y | L | C | D | A | L | Y | D | Y | T |
| H | C | W | L | T | T | S | Y | T | T | T | Y | L | C | D | A | L | Y | D | Y | T |
| I | C | W | L | T | T | S | Y | T | T | T | Y | L | C | D | A | L | Y | D | Y | T |
| J | C | W | L | T | T | S | Y | T | T | T | Y | L | C | D | A | L | Y | D | Y | T |
| K | C | W | L | T | T | S | Y | T | T | T | Y | L | C | D | A | L | Y | D | Y | T |
| L | C | W | L | T | T | S | Y | T | T | T | Y | L | C | D | A | L | Y | D | Y | T |
| M | C | W | L | T | T | S | Y | T | T | T | Y | L | C | D | A | L | Y | D | Y | T |
| N | C | W | L | T | T | S | Y | T | T | T | Y | L | C | D | A | L | Y | D | Y | T |
| O | C | W | L | T | T | S | Y | T | T | T | Y | L | C | D | A | L | Y | D | Y | T |
| P | C | W | L | T | T | S | Y | T | T | T | Y | L | C | D | A | L | Y | D | Y | T |
| Q | C | W | L | T | T | S | Y | T | T | T | Y | L | C | D | A | L | Y | D | Y | T |
| R | C | W | L | T | T | S | Y | T | T | T | Y | L | C | D | A | L | Y | D | Y | T |
| S | C | W | L | T | T | S | Y | T | T | T | Y | L | C | D | A | L | Y | D | Y | T |
| T | C | W | L | T | T | S | Y | T | T | T | Y | L | C | D | A | L | Y | D | Y | T |
| U | C | W | L | T | T | S | Y | T | T | T | Y | L | C | D | A | L | Y | D | Y | T |
| V | C | W | L | T | T | S | Y | T | T | T | Y | L | C | D | A | L | Y | D | Y | T |
| W | C | W | L | T | T | S | Y | T | T | T | Y | L | C | D | A | L | Y | D | Y | T |
| X | C | W | L | T | T | S | Y | T | T | T | Y | L | C | D | A | L | Y | D | Y | T |
| Y | C | W | L | T | T | S | Y | T | T | T | Y | L | C | D | A | L | Y | D | Y | T |
| Z | C | W | L | T | T | S | Y | T | T | T | Y | L | C | D | A | L | Y | D | Y | T |
| AA | C | W | L | T | T | S | Y | T | T | T | Y | L | C | D | A | L | Y | D | Y | T |
| BB | C | W | L | T | T | S | Y | T | T | T | Y | L | C | D | A | L | Y | D | Y | T |
| CC | C | W | L | T | T | S | Y | T | T | T | Y | L | C | D | A | L | Y | D | Y | T |
| DD | C | W | L | T | T | S | Y | T | T | T | Y | L | C | D | A | L | Y | D | Y | T |
| EE | C | W | L | T | T | S | Y | T | T | T | Y | L | C | D | A | L | Y | D | Y | T |
| FF | C | W | L | T | T | S | Y | T | T | T | Y | L | C | D | A | L | Y | D | Y | T |
| GG | C | W | L | T | T | S | Y | T | T | T | Y | L | C | D | A | L | Y | D | Y | T |
| HH | C | W | L | T | T | S | Y | T | T | T | Y | L | C | D | A | L | Y | D | Y | T |
| II | C | W | L | T | T | S | Y | T | T | T | Y | L | C | D | A | L | Y | D | Y | T |
| JJ | C | W | L | T | T | S | Y | T | T | T | Y | L | C | D | A | L | Y | D | Y | T |
| KK | C | W | L | T | T | S | Y | T | T | T | Y | L | C | D | A | L | Y | D | Y | T |
| LL | C | W | L | T | T | S | Y | T | T | T | Y | L | C | D | A | L | Y | D | Y | T |
| MM | C | W | L | T | T | S | Y | T | T | T | Y | L | C | D | A | L | Y | D | Y | T |
| NN | C | W | L | T | T | S | Y | T | T | T | Y | L | C | D | A | L | Y | D | Y | T |
| OO | C | W | L | T | T | S | Y | T | T | T | Y | L | C | D | A | L | Y | D | Y | T |

114. An isolated synthase having a region with 40% or greater sequence identity to residues 309 to 577 of SEQ ID NO: 24, wherein one or more amino acid residues of said synthase that align with amino acids at positions 314, 317, 338, 341, 342, 420, 446, 447, 448, 449, 452, 485, 489, 560, 563, 564, 569, 571 and 572 of SEQ ID NO: 24 are residues other than the following ordered arrangements of residues:

claim 114

| Ordered Arrangement of Residues | | | | | | | | | | | | | | | | | | | |
|---------------------------------|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| A | B | C | D | E | F | G | H | I | J | K | L | M | N | O | P | Q | R | S | T |
| 314 | C | C | G | G | C | G | C | L | P | A | N | C | S | N | C | C | C | C | S |
| 317 | W | W | W | W | W | W | W | W | W | W | W | W | W | W | W | W | W | W | W |
| 338 | I | I | I | I | I | I | I | I | I | I | I | I | I | I | I | I | I | I | I |
| 341 | I | I | I | I | I | I | I | I | I | I | I | I | I | I | I | I | I | I | I |
| 342 | S | S | S | S | S | S | S | S | S | S | S | S | S | S | S | S | S | S | S |
| 420 | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y |
| 446 | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T |
| 447 | T | S | C | S | A | T | A | V | S | T | S | I | S | S | T | G | V | I | S |
| 448 | T | T | G | G | V | G | A | G | C | T | A | S | S | L | G | T | S | A | S |
| 449 | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y |
| 452 | L | L | L | L | L | L | L | L | L | L | L | L | L | L | L | L | L | L | L |
| 485 | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C |
| 489 | D | D | D | D | D | D | D | D | D | D | D | D | D | D | D | D | D | D | D |
| 560 | V | I | M | M | A | A | A | V | A | C | I | A | V | L | A | A | I | A | V |
| 563 | T | T | L | L | L | V | L | L | C | S | T | M | L | S | M | I | T | I | I |
| 564 | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y |
| 569 | D | D | D | D | D | D | D | D | D | D | D | D | D | D | D | D | D | D | D |
| 571 | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y | Y |
| 572 | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T | T |

115. An isolated synthase having a region with 40% or greater sequence identity to residues 315 to 584 of SEQ ID NO: 26, wherein one or more amino acid residues of said synthase that align with amino acids at positions 320, 323, 344, 347, 348, 426, 451, 452, 453, 454, 457, 492, 496, 568, 571, 572, 576, 578 and 579 of SEQ ID NO: 26 are residues other than the following ordered arrangements of residues:

claim 115

Ordered Arrangement of Residues

579 T T T T T T T S T T T S T Q T T G G T G G G G G T S G Y N S S T G T T T T Y T T G G G
578 Y Y Y Y Y Y Y F Y Y F H F F H F Y D H F H F L Y H L Y F F Y Y F F Y Y L Y Y H F F
576 D D D D D D D D D E D D E D
572 Y Y Y Y Y Y Y Y Y Y Y Y Y Y Y Y Y Y Y F Y Y Y Y Y Y Y Y Y Y Y Y Y Y Y Y F Y
571 T T L L L V L L C S T M L S M I T I I I M I F G V I L L M V F F F F S I T T M I I
568 V I M M A A A V A C I A V L A A I A V A S T M F A L L L I F V L L V T L V I A T A
496 D D D D N D N D D N N D G N D D N D N D N D N D N G N D M G D G N N N N N D D D D D D
492 C C C C A G A F S G G L G G L L G L L L F S G L L G C L S L W G G G I G C C L S L
457 L L L L I L L L M T M L L L L T I I I L V S I L T V L I C V I I V L L L M L I
454 Y Y Y Y Y H Y N G I A G Y A P I M A V S S Q L H V M S Y M G L G L L L M Y Y G Q S
453 T T G G G V G A C T S S L G G T S S A S S G A G S G T A G S G L A A G G T T S G A
452 T S C S A T A V T S I I S T S G V I S V I I I C S S L S T S V A F F T S S T I I V
451 T T T T S S S S S T E S S A I I A S S S S S S S S S A S N V S F S S T S T T S S S
426 Y Y Y Y Y Y Y Y F A Y Y N Y Y F Y F Y Y Y Y Y F Y N Y Y F Y M M M Y Y Y Y Y Y
348 S S S S S S S T D G G T T V T T T T V T T T T V T T T T T V T T T T S T S S T T T
347 I I A A T T T T V C L I L L L I V L I I A L Q T I I C L V M V Q T T T T I C I I I Q A
344 I I I I L L L I I V F N V F N N L I F I N A S C F A N C A C G G G G V A I I N A I
323 W W W W W W W W F W W F W W Y W W W L S L S W A L W M S S S A W W W W A A
320 C C G G C G C L P A N C S N C C C C S S N F I Y G Y A F F Y V C C C I Y C C C F F
A B C D E F G H I J K L M N O P Q R S T U V W X Y Z AA BB CC DD EE FF GG HH II JJ KK LL MM NN OO

116. An isolated synthase having a region with 40% or greater sequence identity to residues 265 to 536 of SEQ ID NO: 28, wherein one or more amino acid residues of said synthase that align with amino acids at positions 270, 273, 294, 297, 298, 376, 401, 402, 403, 404, 407, 440, 444, 518, 521, 522, 528, 530 and 531 of SEQ ID NO: 28 are residues other than the following ordered arrangements of residues:

531 T T T T T T S T T S T Q T T G G T G G G G T S G Y N S S T G T T T T Y T T G G G
 530 Y Y Y Y Y Y Y F Y Y F H F F H F Y D H F H F L Y H L Y F F Y Y F F Y Y L Y Y H F F
 528 D D D D D D D D D E D
 522 Y Y Y Y Y Y Y Y Y Y Y Y Y Y Y Y Y Y Y F Y Y Y Y Y Y Y Y Y Y Y Y Y Y Y Y F Y
 521 T T L L L V L L C S T M L S M I T I I I M I F G V I L L M V F F F F S I T T M I I
 518 V I M M A A A V A C I A V L A A I A V A S T M F A L L L I F V L L V T L V I A T A
 444 D D D D N D N D D N N D G N D D N D N D N D N D N G N D M G D G N N N N N D D D D D D
 440 C C C C A G A F S G G L G G L L L G L L L F S G L L G C L S L W G G G I G C C L S L
 Ordered Arrangement of Residues
 407 L L L L I L L L L M T M L L L L T I I I I L V S I L T V L I C V I I V L L L M L I
 404 Y Y Y Y Y H Y N G I A G Y A P I M A V S S Q L H V M S Y M G L G L L L M Y Y G Q S
 403 T T G G G V G G A C T S S L G G T S S A S G A G S G T A G S G L A A G G T T S G A
 402 T S C S A T A V T S I I S T S G V I S V I I I C S S L S T S V A F F T S S T I I V
 401 T T T T S S S S S T E S S A I I A S S S S S S S S A S N V S F S S T S T T S S S
 376 Y Y Y Y Y Y Y Y F A Y Y N Y Y F Y Y Y Y Y Y F Y N Y Y F Y M M M Y Y Y Y Y Y
 298 S S S S S S T D G G T T V T T T T V T T T T T T T T T T T V T T T S T S T T T
 287 I I A A T L T T V C L I L L I V L I I A L Q T I I C L V M V Q T T T I C I I I Q A
 284 I I I I L L L I I V F N V F N N L I F I N A S C F A N C A C G G G G V A I I N A I
 273 W W W W W W W W F W W F W W Y W W W L S L S W A L W M S S S A W W W W A A
 270 C C G G C G C L P A N C S N C C C C S S N F I Y G Y A F F Y V C C C I Y C C C F F
 A B C D E F G H I J K L M N O P Q R S T U V W X Y Z AA BB CC DD EE FF GG HH II JJ KK LL MM NN OO

117. An isolated synthase having a region with 40% or greater sequence identity to residues 342 to 612 of SEQ ID NO: 30, wherein one or more amino acid residues of said synthase that align with amino acids at positions 347, 350, 371, 374, 375, 453, 478, 479, 480, 481, 483, 518, 522, 596, 599, 600, 604, 606 and 607 of SEQ ID NO: 30 are residues other than the following ordered arrangements of residues:

claim 117

| Ordered Arrangement of Residues | | | | | | | | | | | | | | | | | | | |
|---------------------------------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| | 347 | 350 | 371 | 374 | 375 | 453 | 478 | 479 | 480 | 481 | 483 | 518 | 522 | 596 | 599 | 600 | 604 | 606 | 607 |
| A | C | W | I | I | S | Y | T | T | T | Y | L | C | D | V | T | Y | D | Y | T |
| B | C | W | I | I | S | Y | T | S | T | Y | L | C | D | I | T | Y | D | Y | T |
| C | G | W | I | A | S | Y | T | C | G | Y | L | C | D | M | L | Y | D | Y | T |
| D | G | W | L | T | S | Y | S | A | G | Y | L | C | D | A | L | Y | D | Y | T |
| E | C | W | L | T | S | Y | S | A | G | Y | L | C | D | A | L | Y | D | Y | T |
| F | C | W | L | T | S | Y | S | A | G | Y | L | C | D | A | L | Y | D | Y | T |
| G | L | W | I | T | T | Y | S | V | G | Y | L | C | D | A | L | Y | D | Y | T |
| H | P | W | I | V | D | Y | S | T | A | G | L | S | D | A | C | Y | D | Y | T |
| I | A | W | V | C | G | F | T | S | C | I | M | G | N | C | S | Y | D | Y | T |
| J | N | F | F | L | T | Y | E | I | T | A | T | G | N | T | T | Y | D | Y | T |
| K | C | W | N | I | T | Y | S | I | S | G | M | L | D | A | M | Y | D | Y | T |
| L | S | W | V | L | T | Y | S | S | L | Y | L | G | N | A | L | Y | D | Y | T |
| M | N | W | F | L | T | Y | S | T | G | A | L | G | N | A | L | Y | D | Y | T |
| N | C | W | N | I | T | Y | I | S | G | P | L | L | D | A | S | Y | D | Y | T |
| O | C | W | N | V | T | Y | I | G | G | I | L | L | D | A | T | Y | D | Y | T |
| P | C | W | N | L | T | Y | A | V | T | M | L | L | D | A | T | Y | D | Y | T |
| Q | C | W | L | L | T | Y | S | I | S | A | I | L | D | A | T | Y | D | Y | T |
| R | C | W | I | I | T | Y | S | I | S | A | I | L | D | A | T | Y | D | Y | T |
| S | S | W | F | I | T | Y | S | V | A | S | I | L | D | A | T | Y | D | Y | T |
| T | S | W | I | A | T | Y | S | S | A | S | I | L | D | A | T | Y | D | Y | T |
| U | N | W | N | L | T | Y | S | I | S | S | I | F | N | S | T | Y | D | Y | T |
| V | F | L | A | Q | T | Y | S | I | G | Q | L | S | D | T | M | Y | D | Y | T |
| W | L | S | A | T | T | Y | S | I | A | L | V | G | N | F | G | Y | D | Y | T |
| X | Y | L | C | I | T | Y | S | C | G | H | S | L | G | F | V | Y | D | Y | T |
| Y | G | S | F | I | T | Y | S | S | S | V | I | L | D | A | I | Y | D | Y | T |
| Z | Y | W | A | C | T | Y | S | S | G | M | L | C | M | L | L | Y | D | Y | T |
| AA | A | A | N | L | T | N | A | L | T | S | T | C | M | L | L | Y | D | Y | T |
| BB | F | L | C | V | T | Y | S | S | A | Y | V | L | G | L | L | Y | D | Y | T |
| CC | F | W | A | M | T | Y | S | M | G | M | L | S | D | I | M | Y | D | Y | T |
| DD | V | M | C | V | T | Y | V | V | S | G | L | W | N | V | V | Y | D | Y | T |
| EE | V | S | G | Q | T | Y | F | A | G | L | C | N | N | L | F | Y | D | Y | T |
| FF | C | S | G | T | T | M | F | A | L | L | V | G | N | L | F | Y | D | Y | T |
| GG | C | S | G | T | T | M | F | A | L | L | V | G | N | L | F | Y | D | Y | T |
| HH | C | A | G | T | T | M | F | A | L | L | V | G | N | L | F | Y | D | Y | T |
| II | I | W | V | I | S | Y | T | A | G | L | L | I | N | T | S | Y | D | Y | T |
| JJ | Y | W | A | C | T | Y | S | G | G | M | L | G | N | T | S | Y | D | Y | T |
| KK | C | W | I | I | S | Y | T | T | T | Y | L | C | D | V | T | Y | D | Y | T |
| LL | C | W | I | I | S | Y | T | T | T | Y | L | C | D | V | T | Y | D | Y | T |
| MM | C | W | N | I | T | Y | T | T | T | Y | L | C | D | V | T | Y | D | Y | T |
| NN | F | A | A | Q | T | Y | S | I | S | G | M | L | D | A | T | Y | D | Y | T |
| OO | F | A | I | A | T | Y | S | V | A | S | I | L | D | A | T | Y | D | Y | T |

118. An isolated synthase having a region with about 40% or greater sequence identity to residues 307 to 541 of SEQ ID NO: 32, wherein one or more amino acid residues of said synthase that align with amino acids at positions 278, 281, 302, 305, 306, 384, 409, 410, 411, 412, 415, 448, 452, 524, 527, 528, 533, 535 and 536 of SEQ ID NO: 32 are residues other than the following ordered arrangements of residues:

claim 118

| | | Ordered Arrangement of Residues | | | | | | | | | | | | | | | | | | |
|----|---|---------------------------------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| | | 278 | 281 | 302 | 305 | 306 | 384 | 409 | 410 | 411 | 412 | 415 | 448 | 452 | 524 | 527 | 528 | 533 | 535 | 536 |
| A | C | W | I | I | S | S | Y | T | T | T | Y | L | C | D | V | T | Y | D | Y | T |
| B | C | W | I | I | S | S | Y | T | S | T | Y | L | C | D | I | T | Y | D | Y | T |
| C | G | W | I | A | S | S | Y | T | C | G | Y | L | C | D | M | L | Y | D | Y | T |
| D | G | W | L | A | S | S | Y | S | A | G | Y | L | C | D | A | L | Y | D | Y | T |
| E | G | W | L | L | S | S | Y | S | A | G | Y | L | C | D | A | L | Y | D | Y | T |
| F | G | W | L | L | S | S | Y | S | A | G | Y | L | C | D | A | L | Y | D | Y | T |
| G | C | W | L | L | S | S | Y | S | A | G | Y | L | C | D | A | L | Y | D | Y | T |
| H | C | W | L | L | S | S | Y | S | A | G | Y | L | C | D | A | L | Y | D | Y | T |
| I | P | W | I | V | D | G | Y | S | T | A | G | L | F | D | V | C | Y | D | Y | T |
| J | A | W | V | C | G | G | F | S | C | T | A | M | S | D | A | S | Y | D | Y | T |
| K | N | F | L | I | T | T | Y | S | I | T | A | M | S | D | A | S | Y | D | Y | T |
| L | C | W | N | I | T | T | Y | S | I | T | A | M | S | D | A | S | Y | D | Y | T |
| M | S | W | V | L | L | V | N | S | S | S | G | L | G | D | A | V | Y | D | Y | T |
| N | N | F | F | L | T | T | N | A | T | L | A | L | G | D | V | L | Y | D | Y | T |
| O | C | W | N | I | T | T | Y | I | S | G | P | L | L | D | A | M | Y | D | Y | T |
| P | C | W | N | V | T | T | Y | I | S | G | P | L | L | D | A | M | Y | D | Y | T |
| Q | C | Y | L | L | T | T | F | A | V | T | M | T | G | N | A | T | Y | D | Y | T |
| R | C | W | I | I | T | T | Y | S | I | S | A | I | L | D | A | I | Y | D | Y | T |
| S | S | W | F | I | V | T | F | S | S | S | V | I | L | D | A | I | Y | D | Y | T |
| T | S | W | N | A | L | T | Y | S | S | S | V | I | L | D | A | I | Y | D | Y | T |
| U | N | F | L | A | Q | T | Y | S | I | G | Q | L | F | D | A | I | Y | D | Y | T |
| V | F | I | S | S | T | V | Y | S | I | A | L | V | G | N | S | I | F | D | Y | T |
| W | Y | L | S | C | I | T | Y | S | C | G | H | S | L | G | M | F | Y | D | Y | T |
| X | Y | G | S | I | T | T | Y | S | S | G | V | I | L | G | N | A | Y | D | Y | T |
| Y | Y | S | S | I | T | T | Y | S | S | G | V | I | L | G | N | A | Y | D | Y | T |
| Z | Y | W | A | C | T | T | N | A | S | L | T | V | L | D | L | L | Y | D | Y | T |
| AA | A | A | N | L | T | T | Y | S | S | T | A | M | L | G | M | L | Y | D | Y | T |
| BB | F | L | C | V | T | T | Y | S | S | T | A | M | L | G | M | L | Y | D | Y | T |
| CC | F | W | A | M | T | T | Y | S | S | T | A | M | L | G | M | L | Y | D | Y | T |
| DD | V | M | C | V | T | T | Y | S | S | V | G | L | C | N | V | F | Y | D | Y | T |
| EE | V | S | G | Q | T | T | Y | S | S | V | G | L | C | N | V | F | Y | D | Y | T |
| FF | C | S | G | T | T | T | M | S | F | A | L | L | W | N | L | F | Y | D | Y | T |
| GG | C | S | G | T | T | T | M | S | F | A | L | L | W | N | L | F | Y | D | Y | T |
| HH | C | A | V | T | T | T | M | S | F | A | L | L | W | N | L | F | Y | D | Y | T |
| II | I | W | A | C | T | T | Y | S | S | G | M | L | C | D | V | I | Y | D | Y | T |
| JJ | Y | W | A | C | T | T | Y | S | S | G | M | L | C | D | V | I | Y | D | Y | T |
| KK | C | W | I | I | S | S | Y | S | T | T | Y | L | C | D | V | I | Y | D | Y | T |
| LL | C | W | I | I | S | S | Y | S | T | T | Y | L | C | D | V | I | Y | D | Y | T |
| MM | C | W | I | I | S | S | Y | S | T | T | Y | L | C | D | V | I | Y | D | Y | T |
| NN | F | A | A | Q | T | T | Y | S | I | G | Q | L | F | D | A | I | Y | D | Y | T |
| OO | F | A | A | Q | T | T | Y | S | I | G | Q | L | F | D | A | I | Y | D | Y | T |

119. A method for making a terpene synthase, comprising:
- a) identifying, in a preselected polypeptide having a region with 20% or greater sequence identity to residues 265 to 535 of SEQ ID NO: 2, nine amino acid residues whose α -carbons have interatomic distances in Angstroms between said α -carbons that are ± 2.3 Angstroms of the following interatomic distances:

| α -Carbon | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 |
|------------------|------|------|------|------|------|------|------|------|------|
| 1 | 0.0 | 8.4 | 13.7 | 12.7 | 11.9 | 10.2 | 13.1 | 9.4 | 12.8 |
| 2 | 8.4 | 0.0 | 11.3 | 8.7 | 10.2 | 7.2 | 14.8 | 15.1 | 17.4 |
| 3 | 13.7 | 11.3 | 0.0 | 3.8 | 5.4 | 9.3 | 6.6 | 13.9 | 13.7 |
| 4 | 12.7 | 8.7 | 3.8 | 0.0 | 3.8 | 6.0 | 9.2 | 15.4 | 16.1 |
| 5 | 11.9 | 10.2 | 5.4 | 3.8 | 0.0 | 5.0 | 7.8 | 14.6 | 15.5 |
| 6 | 10.2 | 7.2 | 9.3 | 6.0 | 5.0 | 0.0 | 12.0 | 16.1 | 18.0 |
| 7 | 13.1 | 14.8 | 6.6 | 9.2 | 7.8 | 12.0 | 0.0 | 10.2 | 9.5 |
| 8 | 9.4 | 15.1 | 13.9 | 15.4 | 14.6 | 16.1 | 10.2 | 0.0 | 3.8 |
| 9 | 12.8 | 17.4 | 13.7 | 16.1 | 15.5 | 18.0 | 9.5 | 3.8 | 0.0 |

the center point of each said α -carbon positioned within a sphere having a radius of 2.3 Angstroms, the center point of each said sphere having the following structural coordinates:

| α -Carbon Number | X Position | Y Position | Z Position |
|-------------------------|------------|------------|------------|
| 1 | 120.203 | 38.695 | 43.506 |
| 2 | 114.058 | 43.884 | 41.015 |
| 3 | 106.807 | 36.336 | 45.151 |
| 4 | 107.629 | 38.010 | 41.804 |
| 5 | 109.375 | 34.842 | 40.617 |
| 6 | 111.944 | 37.854 | 37.602 |
| 7 | 110.233 | 31.098 | 47.361 |
| 8 | 118.846 | 34.443 | 51.796 |
| 9 | 116.461 | 32.848 | 54.290 |

; and

- b) synthesizing a polypeptide that is modified from said preselected polypeptide, said modified polypeptide having one or more R-groups associated with said α -carbons other than the R-groups associated with said α -carbons in said preselected polypeptide, wherein said modified polypeptide has terpene synthase activity.

120. The method of claim 119, wherein said synthesizing step comprises the formation of a nucleic acid encoding said preselected polypeptide in which the coding sequence for one or more amino acids corresponding to said nine α -carbons is replaced by a coding sequence that codes for an amino acid different from the amino acid present in said preselected polypeptide.

121. The method of claim 119, wherein said preselected polypeptide is a pinene synthase.

122. The method of claim 121, wherein said preselected polypeptide is SEQ ID NO: 20.

123. The method of claim 119, wherein said preselected polypeptide is a taxadiene synthase.

124. The method of claim 123, wherein said preselected polypeptide is SEQ ID NO: 44.

125. A method of using a terpene synthase, comprising:

a) identifying, in a preselected polypeptide having a region with 20% or greater sequence identity to residues 265 to 535 of SEQ ID NO: 2, amino acid residues at nine positions that align with amino acid residues at positions 273, 294, 402, 403, 404, 407, 440, 519 and 520 of SEQ ID NO: 2; and

b) synthesizing a polypeptide that is modified from said preselected polypeptide, said modified polypeptide having amino acid residues at one or more of said nine positions other than the amino acid residues present in said preselected polypeptide.

126. The method of claim 125, wherein said identifying step comprises identifying sixteen amino acid residues in said preselected polypeptide that align with amino acid residues at positions 270, 273, 294, 297, 298, 402, 403, 404, 407, 440, 516, 519, 520, 525, 527 and 528 of SEQ ID NO: 2, and said synthesizing step comprises synthesizing a polypeptide that is modified from said preselected polypeptide, said modified polypeptide having amino acid residues at one or more of said sixteen positions other than the amino acid residues present in said preselected polypeptide.

127. The method of claim 125, wherein said identifying step comprises identifying nineteen amino acid residues in said preselected polypeptide that align with amino acid residues at positions 270, 273, 294, 297, 298, 376, 401, 402, 403, 404, 407, 440, 444, 516, 519, 520, 525, 527 and 528 of SEQ ID NO: 2, and said synthesizing step comprises synthesizing a polypeptide that is modified from said preselected polypeptide, said modified polypeptide having amino acid residues at one or more of said nineteen positions other than the amino acid residues present in said preselected polypeptide.

128. The method of claim 125, wherein said synthesizing step comprises the formation of a nucleic acid encoding said preselected polypeptide in which the coding sequence in said nucleic acid coding for one or more of said nine amino acid residues is replaced by a coding sequence that codes for an amino acid different from the amino acid present in said preselected polypeptide.

129. The method of claim 125, wherein said preselected polypeptide is a pinene synthase.

130. The method of claim 129, wherein said preselected polypeptide is SEQ ID NO: 20.

131. The method of claim 125, wherein said preselected polypeptide is a taxadiene synthase.

132. The method of claim 131, wherein said preselected polypeptide is SEQ ID NO: 44.

133. The method of claim 125, further comprising:
c) contacting said modified polypeptide with a isoprenoid substrate under conditions effective for said substrate to bind said synthase; and
d) measuring the ability of said modified polypeptide to catalyze the formation of a reaction product from said substrate.

134. The method of claim 133, wherein said isoprenoid substrate is a geranyl diphosphate.

135 The method of claim 133, wherein said isoprenoid substrate is a farnesyl diphosphate.

136. The method of claim 133, wherein said isoprenoid substrate is a geranyl genanyl diphosphate.

137. A method of making a terpene synthase, comprising:
creating a population of nucleic acid molecules that encode polypeptides, said population having members that differ from one another at one or more of nine codons specifying amino acids in a region of a preselected terpene synthase polypeptide having 20% or greater sequence identity to residues 265 to 535 of SEQ ID NO: 2, α -carbons of said nine amino acids having interatomic distances in Angstroms between said α -carbons that are ± 2.3 Angstroms of the following interatomic distances:

| α -Carbon | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 |
|------------------|------|------|------|------|------|------|------|------|------|
| 1 | 0.0 | 8.4 | 13.7 | 12.7 | 11.9 | 10.2 | 13.1 | 9.4 | 12.8 |
| 2 | 8.4 | 0.0 | 11.3 | 8.7 | 10.2 | 7.2 | 14.8 | 15.1 | 17.4 |
| 3 | 13.7 | 11.3 | 0.0 | 3.8 | 5.4 | 9.3 | 6.6 | 13.9 | 13.7 |
| 4 | 12.7 | 8.7 | 3.8 | 0.0 | 3.8 | 6.0 | 9.2 | 15.4 | 16.1 |
| 5 | 11.9 | 10.2 | 5.4 | 3.8 | 0.0 | 5.0 | 7.8 | 14.6 | 15.5 |
| 6 | 10.2 | 7.2 | 9.3 | 6.0 | 5.0 | 0.0 | 12.0 | 16.1 | 18.0 |
| 7 | 13.1 | 14.8 | 6.6 | 9.2 | 7.8 | 12.0 | 0.0 | 10.2 | 9.5 |
| 8 | 9.4 | 15.1 | 13.9 | 15.4 | 14.6 | 16.1 | 10.2 | 0.0 | 3.8 |
| 9 | 12.8 | 17.4 | 13.7 | 16.1 | 15.5 | 18.0 | 9.5 | 3.8 | 0.0 |

the center point of each said α -carbon positioned within a sphere having a radius of 2.3 Angstroms, the center point of each said sphere having the following structural coordinates:

| α -Carbon Number | X Position | Y Position | Z Position |
|-------------------------|------------|------------|------------|
| 1 | 120.203 | 38.695 | 43.506 |
| 2 | 114.058 | 43.884 | 41.015 |
| 3 | 106.807 | 36.336 | 45.151 |
| 4 | 107.629 | 38.010 | 41.804 |
| 5 | 109.375 | 34.842 | 40.617 |
| 6 | 111.944 | 37.854 | 37.602 |
| 7 | 110.233 | 31.098 | 47.361 |
| 8 | 118.846 | 34.443 | 51.796 |
| 9 | 116.461 | 32.848 | 54.290 |

; and

b) expressing at least a portion of said nucleic acid population so that a population of polypeptides is made, wherein at least one member of said population of polypeptides is a mutant terpene synthase.

138. The method of claim 137, wherein said expressing step comprises *in vitro* transcription and *in vitro* translation of said nucleic acid populations.

139. The method of claim 137, wherein said expressing step comprises:

- i) cloning said members of said nucleic acid population into an expression vector;
- ii) introducing, into host cells, said cloned nucleic acid population members in said expression vector; and
- iii) expressing said cloned nucleic acid population members in said host cells so that said population of polypeptides is made.

140. The method of claim 139, wherein said host cells are prokaryotic cells.

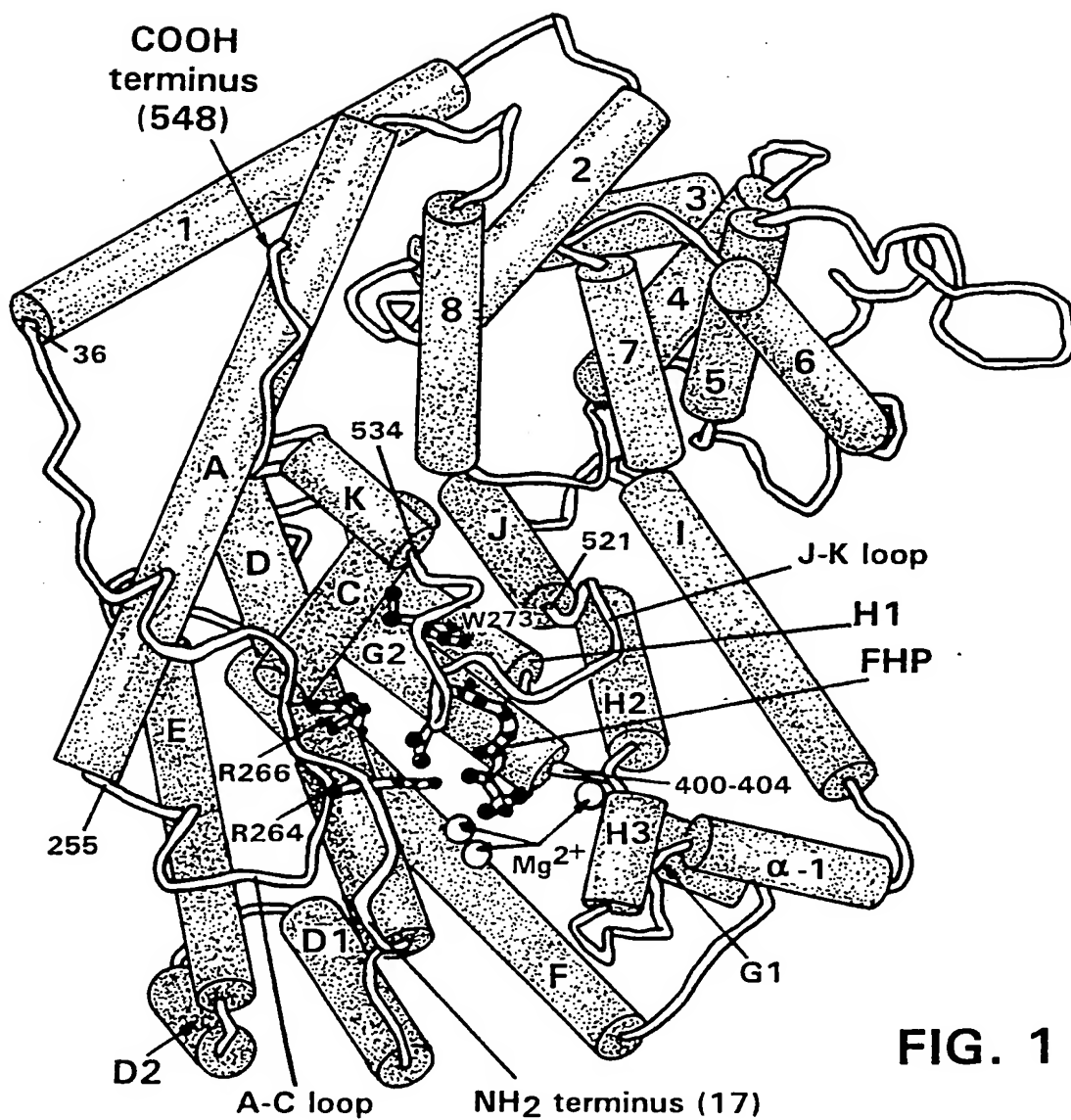
141. The method of claim 137, wherein said preselected terpene synthase polypeptide is a monoterpene synthase.

142. The method of claim 137, wherein said preselected terpene synthase polypeptide is a sesquiterpene synthase.

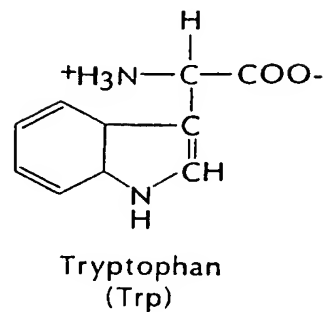
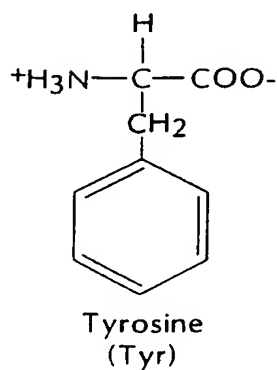
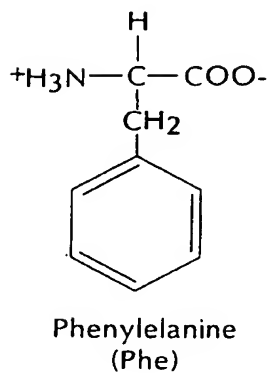
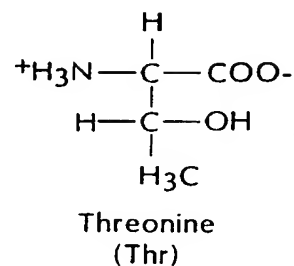
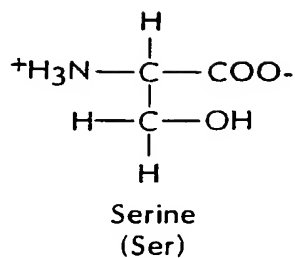
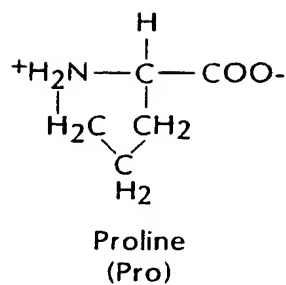
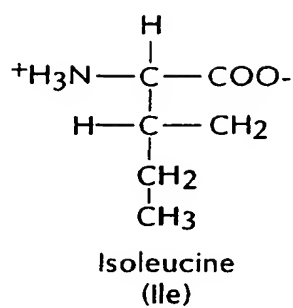
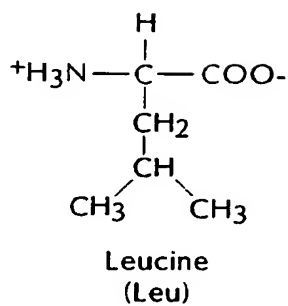
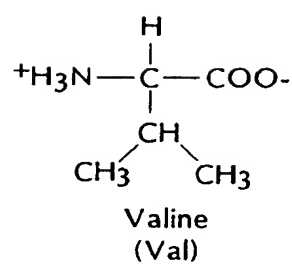
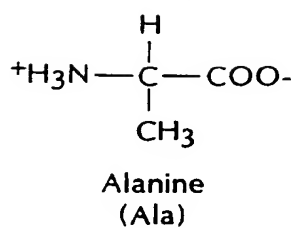
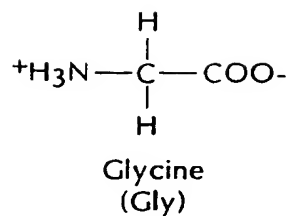
143. The method of claim 137, wherein said preselected terpene synthase polypeptide is a diterpene synthase.
144. An isolated nucleic acid encoding the synthase of claim 1.
145. An isolated nucleic acid encoding the synthase of claim 2.
146. An isolated nucleic acid encoding the synthase of claim 3.
147. An isolated nucleic acid encoding the synthase of claim 7.
148. An isolated nucleic acid encoding a synthase selected from the group consisting of the synthase of claims 11 through 73.
149. An isolated nucleic acid encoding the synthase of claim 80.
150. An isolated nucleic acid encoding the synthase of claim 88.
151. An isolated nucleic acid encoding the synthase of claim 95.
152. An isolated nucleic acid encoding a synthase selected from the group consisting of the synthase of claims 102 through 118.
153. A host cell containing a nucleic acid encoding the synthase of claim 1.
154. The host cell of claim 153, wherein said cell is a prokaryotic cell.
155. The host cell of claim 153, wherein said cell is a eukaryotic cell.
156. The host cell of claim 155, wherein said cell is an insect cell.
157. The host cell of claim 155, wherein said cell is a plant cell.
158. The host cell of claim 157, wherein said host cell is an Angiosperm cell.

159. The host cell of claim 157, wherein said host cell is an Gymnosperm cell.
160. The host cell of claim 157, wherein said host cell is selected from the group consisting of: a cell from a Graminaceae plant, a cell from a Legumineae plant, a cell from a Solanaceae plant, a cell from a Brassicaeae plant and a cell from a Conifereae plant.
161. A transgenic plant containing a nucleic acid encoding the synthase of claim 1.
162. A transgenic animal cell culture containing a nucleic acid encoding the synthase of claim 1.

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**FIG. 2A**

SUBSTITUTE SHEET (RULE 26)

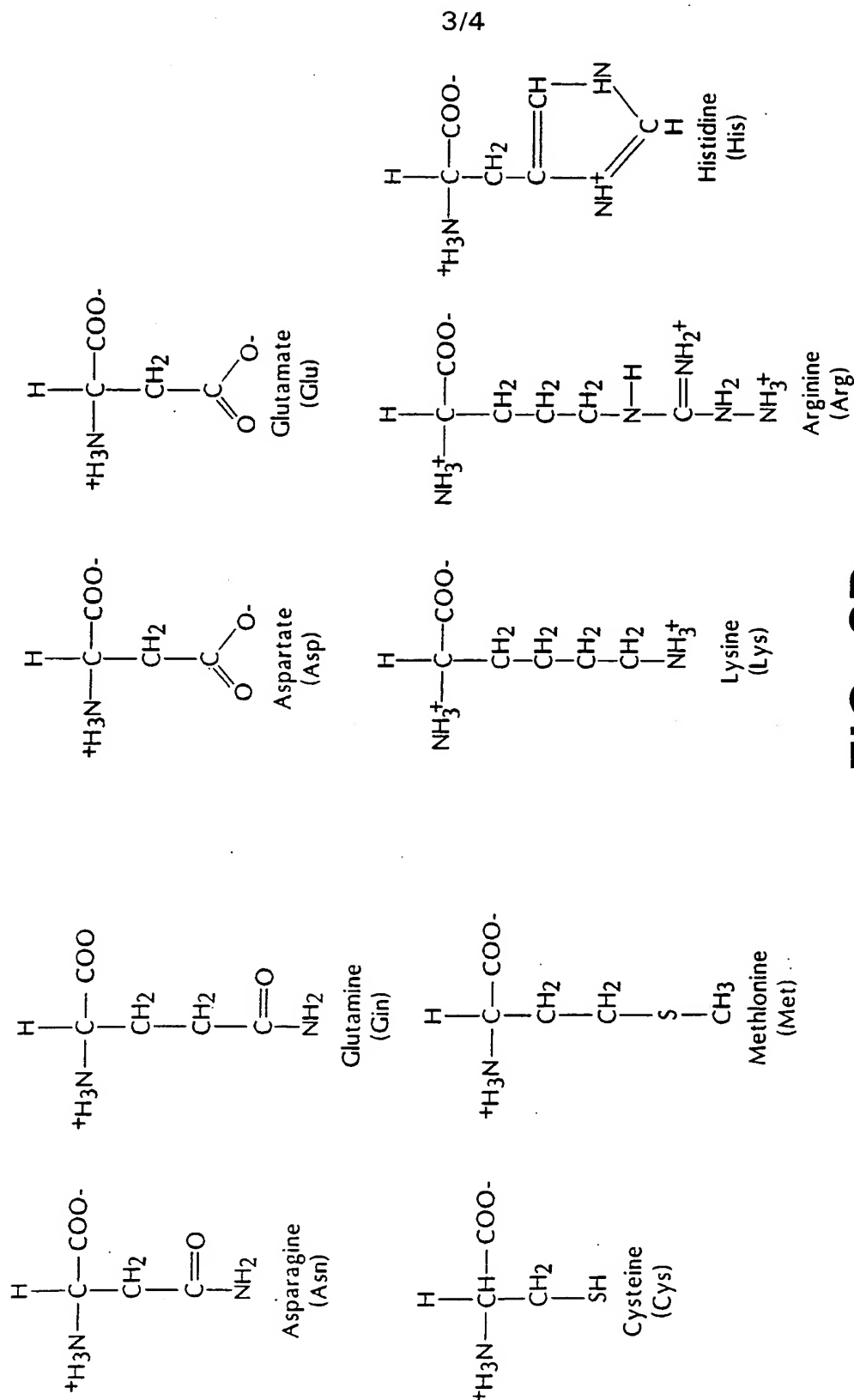


FIG. 2B

4/4

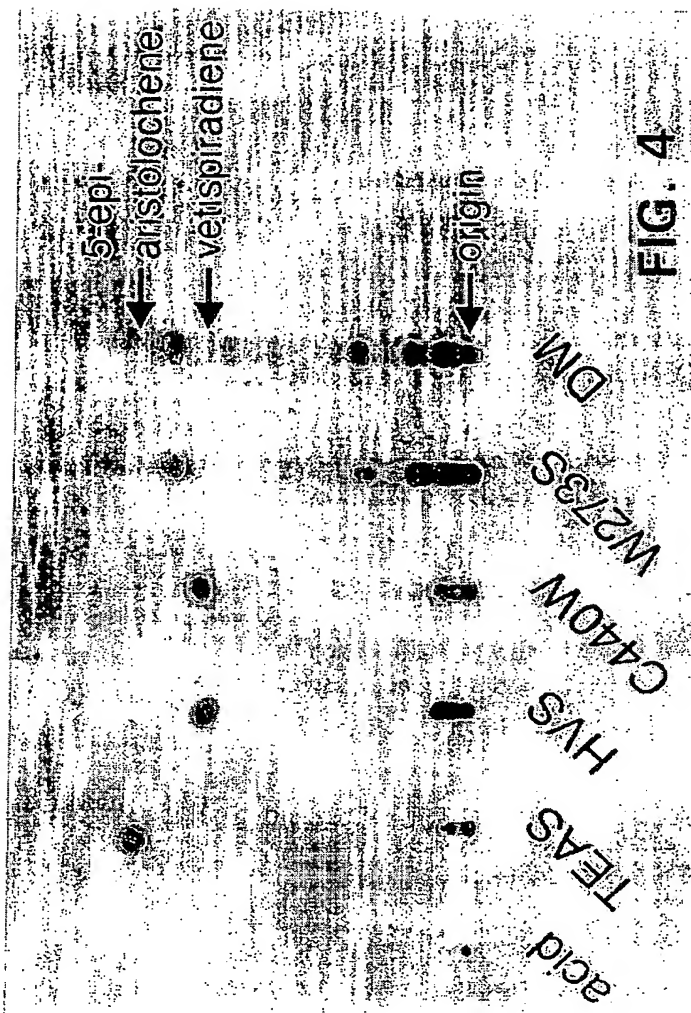


FIG. 4



FIG. 3

SEQUENCE LISTING

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 Noel, Joseph P.
 Starks, Courtney M.
 Manna, Kathleen R.

<120> SYNTHASES

<130> 07678/025W01

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<222> (1)...(1644)

<400> 1

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| gtc gcc gac ttc tcc cct agt ctc tgg ggt gat cag ttc ctt tca ttc | 96 |
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| Ala 65 | Asp | Thr | Leu | Asn 70 | Leu | Ile | Asp | Ile | Ile | Glu 75 | Arg | Leu | Gly | Ile | Ser 80 | |
| tac | cac | ttt | gag | aaa | gaa | att | gat | gag | att | ttg | gat | cag | att | tac | aac | 288 |
| Tyr | His | Phe | Glu | Lys 85 | Glu | Ile | Asp | Glu | Ile 90 | Leu | Asp | Gln | Ile | Tyr | Asn 95 | |
| caa | aac | tca | aac | tgc | aat | gat | ttg | tgc | acc | tct | gca | ctt | caa | ttt | cga | 336 |
| Gln | Asn | Ser | Asn 100 | Cys | Asn | Asp | Leu | Cys 105 | Thr | Ser | Ala | Leu | Gln 110 | Phe | Arg | |
| ttg | ctc | agg | caa | cac | ggc | ttc | aac | atc | tct | cct | gaa | att | ttc | agc | aaa | 384 |
| Leu | Leu | Arg 115 | Gln | His | Gly | Phe | Asn 120 | Ile | Ser | Pro | Glu | Ile 125 | Phe | Ser | Lys | |
| ttc | caa | gat | gaa | aat | ggc | aaa | ttc | aag | gag | tct | ctt | gct | agt | gat | gtc | 432 |
| Phe | Gln 130 | Asp | Glu | Asn | Gly | Lys 135 | Phe | Lys | Glu | Ser | Leu 140 | Ala | Ser | Asp | Val | |
| tta | gga | tta | tta | aac | ttg | tat | gaa | gct | tca | cat | gta | agg | act | cat | gct | 480 |
| Leu | Gly | Leu | Leu | Asn 150 | Leu | Tyr | Glu | Ala | Ser 155 | His | Val | Arg | Thr | His | Ala 160 | |
| gac | gat | atc | tta | gaa | gac | gca | ctt | gct | ttc | tcc | act | atc | cat | ctt | gaa | 528 |
| Asp | Asp | Ile | Leu 165 | Glu | Asp | Ala | Leu | Ala 170 | Phe | Ser | Thr | Ile | His | Leu 175 | Glu | |
| tct | gca | gct | cca | cat | ttg | aaa | tct | cca | ctt | agg | gag | caa | gtg | aca | cat | 576 |
| Ser | Ala | Ala | Pro 180 | His | Leu | Lys | Ser | Pro 185 | Leu | Arg | Glu | Gln | Val 190 | Thr | His | |
| gcc | ctt | gag | caa | tgt | ttg | cac | aag | ggc | ggt | cct | aga | gtc | gag | acc | cga | 624 |
| Ala | Leu 195 | Glu | Gln | Cys | Leu | His | Lys 200 | Gly | Val | Pro | Arg | Val 205 | Glu | Thr | Arg | |
| ttc | ttc | atc | tca | tca | atc | tat | gac | aag | gaa | caa | tcg | aag | aat | aat | gtg | 672 |
| Phe | Phe | Ile | Ser | Ser | Ile | Tyr 215 | Asp | Lys | Glu | Gln 220 | Ser | Lys | Asn | Asn | Val | |
| 210 | | | | | | | | | | | | | | | | |
| tta | ctt | cga | ttt | gcc | aaa | ttg | gat | ttc | aac | ttg | ctc | cag | atg | ttg | cac | 720 |
| Leu | Leu | Arg | Phe | Ala | Lys 230 | Leu | Asp | Phe | Asn 235 | Leu | Leu | Gln | Met | Leu | His 240 | |
| 225 | | | | | | | | | | | | | | | | |
| aaa | caa | gaa | ctt | gct | caa | gta | tca | agg | tgg | tgg | aaa | gat | ttg | gat | ttt | 768 |
| Lys | Gln | Glu | Leu | Ala | Gln | Val | Ser | Arg | Trp 250 | Trp | Lys | Asp | Leu | Asp | Phe 255 | |
| 245 | | | | | | | | | | | | | | | | |
| gta | aca | aca | ctt | cca | tat | gct | aga | gat | cga | gta | ggt | gaa | tgc | tac | ttt | 816 |
| Val | Thr | Thr | Leu 260 | Pro | Tyr | Ala | Arg | Asp 265 | Arg | Val | Val | Glu | Cys | Tyr | Phe | |
| 270 | | | | | | | | | | | | | | | | |
| tgg | gca | tta | gga | ggt | tat | ttt | gag | cct | caa | tac | tct | caa | gct | cgc | gtc | 864 |
| Trp | Ala | Leu | Gly | Val | Tyr | Phe | Glu | Pro | Gln | Tyr | Ser | Gln | Ala | Arg | Val | |

| 275 | | | | | 280 | | | | | 285 | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|
| atg | ctc | ggt | aag | acc | ata | tca | atg | att | tcg | att | gtc | gat | gac | acc | ttt | 912 |
| Met | Leu | Val | Lys | Thr | Ile | Ser | Met | Ile | Ser | Ile | Val | Asp | Asp | Thr | Phe | |
| | 290 | | | | | 295 | | | | | 300 | | | | | |
| gat | gct | tac | ggt | aca | ggt | aaa | gaa | ctt | gag | gca | tac | aca | gat | gcc | ata | 960 |
| Asp | Ala | Tyr | Gly | Thr | Val | Lys | Glu | Leu | Glu | Ala | Tyr | Thr | Asp | Ala | Ile | |
| 305 | | | | | 310 | | | | | 315 | | | | | 320 | |
| caa | aga | tgg | gat | atc | aac | gaa | att | gat | cgg | ctt | cct | gat | tac | atg | aaa | 1008 |
| Gln | Arg | Trp | Asp | Ile | Asn | Glu | Ile | Asp | Arg | Leu | Pro | Asp | Tyr | Met | Lys | |
| | | | | 325 | | | | | 330 | | | | | 335 | | |
| atc | agt | tat | aaa | gct | att | cta | gat | ctc | tac | aag | gat | tat | gaa | aag | gaa | 1056 |
| Ile | Ser | Tyr | Lys | Ala | Ile | Leu | Asp | Leu | Tyr | Lys | Asp | Tyr | Glu | Lys | Glu | |
| | | | 340 | | | | | 345 | | | | | 350 | | | |
| ttg | tct | agt | gcc | gga | aga | tct | cat | att | gtc | tgc | cat | gca | ata | gaa | aga | 1104 |
| Leu | Ser | Ser | Ala | Gly | Arg | Ser | His | Ile | Val | Cys | His | Ala | Ile | Glu | Arg | |
| | | 355 | | | | | 360 | | | | | 365 | | | | |
| atg | aaa | gaa | gta | gta | aga | aat | tat | aat | gtc | gag | tca | aca | tgg | ttt | att | 1152 |
| Met | Lys | Glu | Val | Val | Arg | Asn | Tyr | Asn | Val | Glu | Ser | Thr | Trp | Phe | Ile | |
| | 370 | | | | | 375 | | | | | 380 | | | | | |
| gaa | gga | tat | atg | cca | cct | ggt | tct | gaa | tac | cta | agc | aat | gca | cta | gca | 1200 |
| Glu | Gly | Tyr | Met | Pro | Pro | Val | Ser | Glu | Tyr | Leu | Ser | Asn | Ala | Leu | Ala | |
| 385 | | | | | 390 | | | | | 395 | | | | | 400 | |
| act | acc | aca | tat | tac | tac | ctc | gcg | aca | aca | tcg | tat | ttg | ggc | atg | aag | 1248 |
| Thr | Thr | Thr | Tyr | Tyr | Tyr | Leu | Ala | Thr | Thr | Ser | Tyr | Leu | Gly | Met | Lys | |
| | | | | 405 | | | | | 410 | | | | | 415 | | |
| tct | gcc | acg | gag | caa | gat | ttt | gag | tgg | ttg | tca | aag | aat | cca | aaa | att | 1296 |
| Ser | Ala | Thr | Glu | Gln | Asp | Phe | Glu | Trp | Leu | Ser | Lys | Asn | Pro | Lys | Ile | |
| | | | 420 | | | | 425 | | | | | | 430 | | | |
| ctt | gaa | gct | agt | gta | att | ata | tgt | cga | ggt | atc | gat | gac | aca | gcc | acg | 1344 |
| Leu | Glu | Ala | Ser | Val | Ile | Ile | Cys | Arg | Val | Ile | Asp | Asp | Thr | Ala | Thr | |
| | | 435 | | | | | 440 | | | | | 445 | | | | |
| tac | gag | ggt | gag | aaa | agc | agg | gga | caa | att | gca | act | gga | att | gag | tgc | 1392 |
| Tyr | Glu | Val | Glu | Lys | Ser | Arg | Gly | Gln | Ile | Ala | Thr | Gly | Ile | Glu | Cys | |
| | 450 | | | | | 455 | | | | | 460 | | | | | |
| tgc | atg | aga | gat | tat | ggt | ata | tca | aca | aaa | gag | gca | atg | gct | aaa | ttt | 1440 |
| Cys | Met | Arg | Asp | Tyr | Gly | Ile | Ser | Thr | Lys | Glu | Ala | Met | Ala | Lys | Phe | |
| 465 | | | | | 470 | | | | | 475 | | | | | 480 | |
| caa | aat | atg | gct | gag | aca | gca | tgg | aaa | gat | att | aat | gaa | gga | ctt | ctt | 1488 |
| Gln | Asn | Met | Ala | Glu | Thr | Ala | Trp | Lys | Asp | Ile | Asn | Glu | Gly | Leu | Leu | |
| | | | | 485 | | | | | 490 | | | | | 495 | | |

```

agg ccc act ccc gtc tct aca gaa ttt tta act cct att ctc aat ctt      1536
Arg Pro Thr Pro Val Ser Thr Glu Phe Leu Thr Pro Ile Leu Asn Leu
                    500                    505                    510

gct cgt att gtt gag gtt aca tat ata cac aat cta gat gga tac act      1584
Ala Arg Ile Val Glu Val Thr Tyr Ile His Asn Leu Asp Gly Tyr Thr
                    515                    520                    525

cat ccg gag aaa gtc tta aaa cct cac att att aac cta ctt gtg gac      1632
His Pro Glu Lys Val Leu Lys Pro His Ile Ile Asn Leu Leu Val Asp
                    530                    535                    540

tcc atc aaa att
Ser Ile Lys Ile
545

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<212> PRT
<213> TEAS Native

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Val Ala Asp Phe Ser Pro Ser Leu Trp Gly Asp Gln Phe Leu Ser Phe
      20      25      30
Ser Ile Asp Asn Gln Val Ala Glu Lys Tyr Ala Gln Glu Ile Glu Ala
      35      40      45
Leu Lys Glu Gln Thr Arg Ser Met Leu Leu Ala Thr Gly Arg Lys Leu
      50      55      60
Ala Asp Thr Leu Asn Leu Ile Asp Ile Ile Glu Arg Leu Gly Ile Ser
      65      70      75      80
Tyr His Phe Glu Lys Glu Ile Asp Glu Ile Leu Asp Gln Ile Tyr Asn
      85      90      95
Gln Asn Ser Asn Cys Asn Asp Leu Cys Thr Ser Ala Leu Gln Phe Arg
      100     105     110
Leu Leu Arg Gln His Gly Phe Asn Ile Ser Pro Glu Ile Phe Ser Lys
      115     120     125
Phe Gln Asp Glu Asn Gly Lys Phe Lys Glu Ser Leu Ala Ser Asp Val
      130     135     140
Leu Gly Leu Leu Asn Leu Tyr Glu Ala Ser His Val Arg Thr His Ala
      145     150     155     160
Asp Asp Ile Leu Glu Asp Ala Leu Ala Phe Ser Thr Ile His Leu Glu
      165     170     175
Ser Ala Ala Pro His Leu Lys Ser Pro Leu Arg Glu Gln Val Thr His
      180     185     190
Ala Leu Glu Gln Cys Leu His Lys Gly Val Pro Arg Val Glu Thr Arg
      195     200     205
Phe Phe Ile Ser Ser Ile Tyr Asp Lys Glu Gln Ser Lys Asn Asn Val
      210     215     220
Leu Leu Arg Phe Ala Lys Leu Asp Phe Asn Leu Leu Gln Met Leu His

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225          230          235          240
Lys Gln Glu Leu Ala Gln Val Ser Arg Trp Trp Lys Asp Leu Asp Phe
245          250          255
Val Thr Thr Leu Pro Tyr Ala Arg Asp Arg Val Val Glu Cys Tyr Phe
260          265          270
Trp Ala Leu Gly Val Tyr Phe Glu Pro Gln Tyr Ser Gln Ala Arg Val
275          280          285
Met Leu Val Lys Thr Ile Ser Met Ile Ser Ile Val Asp Asp Thr Phe
290          295          300
Asp Ala Tyr Gly Thr Val Lys Glu Leu Glu Ala Tyr Thr Asp Ala Ile
305          310          315          320
Gln Arg Trp Asp Ile Asn Glu Ile Asp Arg Leu Pro Asp Tyr Met Lys
325          330          335
Ile Ser Tyr Lys Ala Ile Leu Asp Leu Tyr Lys Asp Tyr Glu Lys Glu
340          345          350
Leu Ser Ser Ala Gly Arg Ser His Ile Val Cys His Ala Ile Glu Arg
355          360          365
Met Lys Glu Val Val Arg Asn Tyr Asn Val Glu Ser Thr Trp Phe Ile
370          375          380
Glu Gly Tyr Met Pro Pro Val Ser Glu Tyr Leu Ser Asn Ala Leu Ala
385          390          395          400
Thr Thr Thr Tyr Tyr Tyr Leu Ala Thr Thr Ser Tyr Leu Gly Met Lys
405          410          415
Ser Ala Thr Glu Gln Asp Phe Glu Trp Leu Ser Lys Asn Pro Lys Ile
420          425          430
Leu Glu Ala Ser Val Ile Ile Cys Arg Val Ile Asp Asp Thr Ala Thr
435          440          445
Tyr Glu Val Glu Lys Ser Arg Gly Gln Ile Ala Thr Gly Ile Glu Cys
450          455          460
Cys Met Arg Asp Tyr Gly Ile Ser Thr Lys Glu Ala Met Ala Lys Phe
465          470          475          480
Gln Asn Met Ala Glu Thr Ala Trp Lys Asp Ile Asn Glu Gly Leu Leu
485          490          495
Arg Pro Thr Pro Val Ser Thr Glu Phe Leu Thr Pro Ile Leu Asn Leu
500          505          510
Ala Arg Ile Val Glu Val Thr Tyr Ile His Asn Leu Asp Gly Tyr Thr
515          520          525
His Pro Glu Lys Val Leu Lys Pro His Ile Ile Asn Leu Leu Val Asp
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Ser Ile Lys Ile
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<210> 3
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48

| | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| Met | Ala | Ser | Ala | Ala | Val | Ala | Asn | Tyr | Glu | Glu | Glu | Ile | Val | Arg | Pro | |
| 1 | | | | 5 | | | | | 10 | | | | | 15 | | |
| gtc | gcc | gac | ttc | tcc | cct | agt | ctc | tgg | ggg | gat | cag | ttc | ctt | tca | ttc | 96 |
| Val | Ala | Asp | Phe | Ser | Pro | Ser | Leu | Trp | Gly | Asp | Gln | Phe | Leu | Ser | Phe | |
| | | | 20 | | | | | 25 | | | | | 30 | | | |
| tcc | att | gat | aat | cag | gtt | gcg | gaa | aag | tat | gct | caa | gag | att | gaa | gca | 144 |
| Ser | Ile | Asp | Asn | Gln | Val | Ala | Glu | Lys | Tyr | Ala | Gln | Glu | Ile | Glu | Ala | |
| | | 35 | | | | | 40 | | | | | 45 | | | | |
| ttg | aag | gaa | caa | acg | agg | agt | atg | ctg | tta | gca | acc | gga | agg | aaa | ttg | 192 |
| Leu | Lys | Glu | Gln | Thr | Arg | Ser | Met | Leu | Leu | Ala | Thr | Gly | Arg | Lys | Leu | |
| | 50 | | | | | 55 | | | | | 60 | | | | | |
| gcc | gat | aca | ttg | aat | ttg | att | gac | att | att | gaa | cgc | ctt | ggg | ata | tcc | 240 |
| Ala | Asp | Thr | Leu | Asn | Leu | Ile | Asp | Ile | Ile | Glu | Arg | Leu | Gly | Ile | Ser | |
| 65 | | | | | 70 | | | | | 75 | | | | | 80 | |
| tac | cac | ttt | gag | aaa | gaa | att | gat | gag | att | ttg | gat | cag | att | tac | aac | 288 |
| Tyr | His | Phe | Glu | Lys | Glu | Ile | Asp | Glu | Ile | Leu | Asp | Gln | Ile | Tyr | Asn | |
| | | | 85 | | | | | 90 | | | | | 95 | | | |
| caa | aac | tca | aac | tgc | aat | gat | ttg | tgc | acc | tct | gca | ctt | caa | ttt | cga | 336 |
| Gln | Asn | Ser | Asn | Cys | Asn | Asp | Leu | Cys | Thr | Ser | Ala | Leu | Gln | Phe | Arg | |
| | | | 100 | | | | | 105 | | | | | 110 | | | |
| ttg | ctc | agg | caa | cac | ggg | ttc | aac | atc | tct | cct | gaa | att | ttc | agc | aaa | 384 |
| Leu | Leu | Arg | Gln | His | Gly | Phe | Asn | Ile | Ser | Pro | Glu | Ile | Phe | Ser | Lys | |
| | | 115 | | | | | 120 | | | | | 125 | | | | |
| ttc | caa | gat | gaa | aat | ggc | aaa | ttc | aag | gag | tct | ctt | gct | agt | gat | gtc | 432 |
| Phe | Gln | Asp | Glu | Asn | Gly | Lys | Phe | Lys | Glu | Ser | Leu | Ala | Ser | Asp | Val | |
| | 130 | | | | | 135 | | | | | 140 | | | | | |
| tta | gga | tta | tta | aac | ttg | tat | gaa | gct | tca | cat | gta | agg | act | cat | gct | 480 |
| Leu | Gly | Leu | Leu | Asn | Leu | Tyr | Glu | Ala | Ser | His | Val | Arg | Thr | His | Ala | |
| 145 | | | | | 150 | | | | 155 | | | | | | 160 | |
| gac | gat | atc | tta | gaa | gac | gca | ctt | gct | ttc | tcc | act | atc | cat | ctt | gaa | 528 |
| Asp | Asp | Ile | Leu | Glu | Asp | Ala | Leu | Ala | Phe | Ser | Thr | Ile | His | Leu | Glu | |
| | | | | 165 | | | | | 170 | | | | | 175 | | |
| tct | gca | gct | cca | cat | ttg | aaa | tct | cca | ctt | agg | gag | caa | gtg | aca | cat | 576 |
| Ser | Ala | Ala | Pro | His | Leu | Lys | Ser | Pro | Leu | Arg | Glu | Gln | Val | Thr | His | |
| | | | 180 | | | | | 185 | | | | | 190 | | | |
| gcc | ctt | gag | caa | tgt | ttg | cac | aag | ggg | gtt | cct | aga | gtc | gag | acc | cga | 624 |
| Ala | Leu | Glu | Gln | Cys | Leu | His | Lys | Gly | Val | Pro | Arg | Val | Glu | Thr | Arg | |
| | | 195 | | | | | 200 | | | | | 205 | | | | |
| ttc | ttc | atc | tca | tca | atc | tat | gac | aag | gaa | caa | tcg | aag | aat | aat | gtg | 672 |
| Phe | Phe | Ile | Ser | Ser | Ile | Tyr | Asp | Lys | Glu | Gln | Ser | Lys | Asn | Asn | Val | |

| 210 | 215 | 220 | |
|---|-----|-----|------|
| tta ctt cga ttt gcc aaa ttg gat ttc aac ttg ctc cag atg ttg cac Leu Leu Arg Phe Ala Lys Leu Asp Phe Asn Leu Leu Gln Met Leu His 225 230 235 240 | | | 720 |
| aaa caa gaa ctt gct caa gta tca agg tgg tgg aaa gat ttg gat ttt Lys Gln Glu Leu Ala Gln Val Ser Arg Trp Trp Lys Asp Leu Asp Phe 245 250 255 | | | 768 |
| gta aca aca ctt cca tat gct aga gat cga gta gtt gaa tgc tac ttt Val Thr Thr Leu Pro Tyr Ala Arg Asp Arg Val Val Glu Cys Tyr Phe 260 265 270 | | | 816 |
| gag gca tta gga gtt tat ttt gag cct caa tac tct caa gct cgc gtc Glu Ala Leu Gly Val Tyr Phe Glu Pro Gln Tyr Ser Gln Ala Arg Val 275 280 285 | | | 864 |
| atg ctc gtt aag acc ata tca atg att tcg att gtc gat gac acc ttt Met Leu Val Lys Thr Ile Ser Met Ile Ser Ile Val Asp Asp Thr Phe 290 295 300 | | | 912 |
| gat gct tac ggt aca gtt aaa gaa ctt gag gca tac aca gat gcc ata Asp Ala Tyr Gly Thr Val Lys Glu Leu Glu Ala Tyr Thr Asp Ala Ile 305 310 315 320 | | | 960 |
| caa aga tgg gat atc aac gaa att gat cgg ctt cct gat tac atg aaa Gln Arg Trp Asp Ile Asn Glu Ile Asp Arg Leu Pro Asp Tyr Met Lys 325 330 335 | | | 1008 |
| atc agt tat aaa gct att cta gat ctc tac aag gat tat gaa aag gaa Ile Ser Tyr Lys Ala Ile Leu Asp Leu Tyr Lys Asp Tyr Glu Lys Glu 340 345 350 | | | 1056 |
| ttg tct agt gcc gga aga tct cat att gtc tgc cat gca ata gaa aga Leu Ser Ser Ala Gly Arg Ser His Ile Val Cys His Ala Ile Glu Arg 355 360 365 | | | 1104 |
| atg aaa gaa gta gta aga aat tat aat gtc gag tca aca tgg ttt att Met Lys Glu Val Val Arg Asn Tyr Asn Val Glu Ser Thr Trp Phe Ile 370 375 380 | | | 1152 |
| gaa gga tat atg cca cct gtt tct gaa tac cta agc aat gca cta gca Glu Gly Tyr Met Pro Pro Val Ser Glu Tyr Leu Ser Asn Ala Leu Ala 385 390 395 400 | | | 1200 |
| act acc aca tat tac tac ctc gcg aca aca tcg tat ttg ggc atg aag Thr Thr Thr Tyr Tyr Tyr Leu Ala Thr Thr Ser Tyr Leu Gly Met Lys 405 410 415 | | | 1248 |
| tct gcc acg gag caa gat ttt gag tgg ttg tca aag aat cca aaa att Ser Ala Thr Glu Gln Asp Phe Glu Trp Leu Ser Lys Asn Pro Lys Ile 420 425 430 | | | 1296 |

| | |
|---|------|
| ctt gaa gct agt gta att ata tgt cga gtt atc gat gac aca gcc acg | 1344 |
| Leu Glu Ala Ser Val Ile Ile Cys Arg Val Ile Asp Asp Thr Ala Thr | |
| 435 440 445 | |
| tac gag gtt gag aaa agc agg gga caa att gca act gga att gag tgc | 1392 |
| Tyr Glu Val Glu Lys Ser Arg Gly Gln Ile Ala Thr Gly Ile Glu Cys | |
| 450 455 460 | |
| tgc atg aga gat tat ggt ata tca aca aaa gag gca atg gct aaa ttt | 1440 |
| Cys Met Arg Asp Tyr Gly Ile Ser Thr Lys Glu Ala Met Ala Lys Phe | |
| 465 470 475 480 | |
| caa aat atg gct gag aca gca tgg aaa gat att aat gaa gga ctt ctt | 1488 |
| Gln Asn Met Ala Glu Thr Ala Trp Lys Asp Ile Asn Glu Gly Leu Leu | |
| 485 490 495 | |
| agg ccc act ccc gtc tct aca gaa ttt tta act cct att ctc aat ctt | 1536 |
| Arg Pro Thr Pro Val Ser Thr Glu Phe Leu Thr Pro Ile Leu Asn Leu | |
| 500 505 510 | |
| gct cgt att gtt gag gtt aca tat ata cac aat cta gat gga tac act | 1584 |
| Ala Arg Ile Val Glu Val Thr Tyr Ile His Asn Leu Asp Gly Tyr Thr | |
| 515 520 525 | |
| cat ccg gag aaa gtc tta aaa cct cac att att aac cta ctt gtg gac | 1632 |
| His Pro Glu Lys Val Leu Lys Pro His Ile Ile Asn Leu Leu Val Asp | |
| 530 535 540 | |
| tcc atc aaa att | 1644 |
| Ser Ile Lys Ile | |
| 545 | |

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 20 25 30
 Ser Ile Asp Asn Gln Val Ala Glu Lys Tyr Ala Gln Glu Ile Glu Ala
 35 40 45
 Leu Lys Glu Gln Thr Arg Ser Met Leu Leu Ala Thr Gly Arg Lys Leu
 50 55 60
 Ala Asp Thr Leu Asn Leu Ile Asp Ile Ile Glu Arg Leu Gly Ile Ser
 65 70 75 80
 Tyr His Phe Glu Lys Glu Ile Asp Glu Ile Leu Asp Gln Ile Tyr Asn
 85 90 95
 Gln Asn Ser Asn Cys Asn Asp Leu Cys Thr Ser Ala Leu Gln Phe Arg

| | | | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| Leu | Leu | Arg | 100 | Gln | His | Gly | Phe | Asn | 105 | Ile | Ser | Pro | Glu | Ile | 110 | Phe | Ser | Lys |
| | | 115 | | | | | | 120 | | | | | | 125 | | | | |
| Phe | Gln | Asp | Glu | Asn | Gly | Lys | Phe | Lys | Glu | Ser | Leu | Ala | Ser | Asp | Val | | | |
| | 130 | | | | | 135 | | | | | | 140 | | | | | | |
| Leu | Gly | Leu | Leu | Asn | Leu | Tyr | Glu | Ala | Ser | His | Val | Arg | Thr | His | Ala | | | |
| 145 | | | | | 150 | | | | | 155 | | | | | 160 | | | |
| Asp | Asp | Ile | Leu | Glu | Asp | Ala | Leu | Ala | Phe | Ser | Thr | Ile | His | Leu | Glu | | | |
| | | | 165 | | | | | | 170 | | | | | 175 | | | | |
| Ser | Ala | Ala | Pro | His | Leu | Lys | Ser | Pro | Leu | Arg | Glu | Gln | Val | Thr | His | | | |
| | | 180 | | | | | | 185 | | | | | 190 | | | | | |
| Ala | Leu | Glu | Gln | Cys | Leu | His | Lys | Gly | Val | Pro | Arg | Val | Glu | Thr | Arg | | | |
| | 195 | | | | | | 200 | | | | | 205 | | | | | | |
| Phe | Phe | Ile | Ser | Ser | Ile | Tyr | Asp | Lys | Glu | Gln | Ser | Lys | Asn | Asn | Val | | | |
| | 210 | | | | 215 | | | | | 220 | | | | | | | | |
| Leu | Leu | Arg | Phe | Ala | Lys | Leu | Asp | Phe | Asn | Leu | Leu | Gln | Met | Leu | His | | | |
| 225 | | | | | 230 | | | | 235 | | | | | 240 | | | | |
| Lys | Gln | Glu | Leu | Ala | Gln | Val | Ser | Arg | Trp | Trp | Lys | Asp | Leu | Asp | Phe | | | |
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| Ser | Ala | Thr | Glu | Gln | Asp | Phe | Glu | Trp | Leu | Ser | Lys | Asn | Pro | Lys | Ile | | | |
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 Val Ala Asp Phe Ser Pro Ser Leu Trp Gly Asp Gln Phe Leu Ser Phe
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 Ser Ile Asp Asn Gln Val Ala Glu Lys Tyr Ala Gln Glu Ile Glu Ala
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 Leu Lys Glu Gln Thr Arg Ser Met Leu Leu Ala Thr Gly Arg Lys Leu
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 Tyr His Phe Glu Lys Glu Ile Asp Glu Ile Leu Asp Gln Ile Tyr Asn
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 Gln Asn Ser Asn Cys Asn Asp Leu Cys Thr Ser Ala Leu Gln Phe Arg
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 Leu Leu Arg Gln His Gly Phe Asn Ile Ser Pro Glu Ile Phe Ser Lys
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 Phe Gln Asp Glu Asn Gly Lys Phe Lys Glu Ser Leu Ala Ser Asp Val
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 Leu Gly Leu Leu Asn Leu Tyr Glu Ala Ser His Val Arg Thr His Ala

| 145 | | 150 | | 155 | | 160 | |
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| Asp Asp Ile Leu Glu Asp Ala Leu Ala Phe Ser Thr Ile His Leu Glu | | | | | | | |
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| tct gca gct cca cat ttg aaa tct cca ctt agg gag caa gtg aca cat | | | | | | | 576 |
| Ser Ala Ala Pro His Leu Lys Ser Pro Leu Arg Glu Gln Val Thr His | | | | | | | |
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| Ala Leu Glu Gln Cys Leu His Lys Gly Val Pro Arg Val Glu Thr Arg | | | | | | | |
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| ttc ttc atc tca tca atc tat gac aag gaa caa tcg aag aat aat gtg | | | | | | | 672 |
| Phe Phe Ile Ser Ser Ile Tyr Asp Lys Glu Gln Ser Lys Asn Asn Val | | | | | | | |
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| Leu Leu Arg Phe Ala Lys Leu Asp Phe Asn Leu Leu Gln Met Leu His | | | | | | | |
| | | 225 | | 230 | | 235 | 240 |
| aaa caa gaa ctt gct caa gta tca agg tgg tgg aaa gat ttg gat ttt | | | | | | | 768 |
| Lys Gln Glu Leu Ala Gln Val Ser Arg Trp Trp Lys Asp Leu Asp Phe | | | | | | | |
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| gta aca aca ctt cca tat gct aga gat cga gta gtt gaa tgc tac ttt | | | | | | | 816 |
| Val Thr Thr Leu Pro Tyr Ala Arg Asp Arg Val Val Glu Cys Tyr Phe | | | | | | | |
| | | 260 | | 265 | | 270 | |
| tgg gca tta gga gtt tat ttt gag cct caa tac tct caa gct cgc gtc | | | | | | | 864 |
| Trp Ala Leu Gly Val Tyr Phe Glu Pro Gln Tyr Ser Gln Ala Arg Val | | | | | | | |
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| Met Leu Val Lys Thr Ile Ser Met Ile Ser Ile Val Asp Asp Thr Phe | | | | | | | |
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| gat gct tac ggt aca gtt aaa gaa ctt gag gca tac aca gat gcc ata | | | | | | | 960 |
| Asp Ala Tyr Gly Thr Val Lys Glu Leu Glu Ala Tyr Thr Asp Ala Ile | | | | | | | |
| | | 305 | | 310 | | 315 | 320 |
| caa aga tgg gat atc aac gaa att gat cgg ctt cct gat tac atg aaa | | | | | | | 1008 |
| Gln Arg Trp Asp Ile Asn Glu Ile Asp Arg Leu Pro Asp Tyr Met Lys | | | | | | | |
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| atc agt tat aaa gct att cta gat ctc tac aag gat tat gaa aag gaa | | | | | | | 1056 |
| Ile Ser Tyr Lys Ala Ile Leu Asp Leu Tyr Lys Asp Tyr Glu Lys Glu | | | | | | | |
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| Leu Ser Ser Ala Gly Arg Ser His Ile Val Cys His Ala Ile Glu Arg | | | | | | | |
| | | 355 | | 360 | | 365 | |

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| Glu | Gly | Tyr | Met | Pro | Pro | Val | Ser | Glu | Tyr | Leu | Ser | Asn | Ala | Leu | Ala | |
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| Thr | Thr | Thr | Tyr | Tyr | Tyr | Leu | Ala | Thr | Thr | Ser | Tyr | Leu | Gly | Met | Lys | |
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| tac | gag | gtt | gag | aaa | agc | agg | gga | caa | att | gca | act | gga | att | gag | tgc | 1392 |
| Tyr | Glu | Val | Glu | Lys | Ser | Arg | Gly | Gln | Ile | Ala | Thr | Gly | Ile | Glu | Cys | |
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| Cys | Met | Arg | Asp | Tyr | Gly | Ile | Ser | Thr | Lys | Glu | Ala | Met | Ala | Lys | Phe | |
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| Gln | Asn | Met | Ala | Glu | Thr | Ala | Trp | Lys | Asp | Ile | Asn | Glu | Gly | Leu | Leu | |
| | | | | 485 | | | | | 490 | | | | | 495 | | |
| agg | ccc | act | ccc | gtc | tct | aca | gaa | ttt | tta | act | cct | att | ctc | aat | ctt | 1536 |
| Arg | Pro | Thr | Pro | Val | Ser | Thr | Glu | Phe | Leu | Thr | Pro | Ile | Leu | Asn | Leu | |
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Ala Asp Thr Leu Asn Leu Ile Asp Ile Ile Glu Arg Leu Gly Ile Ser
      65      70      75      80
Tyr His Phe Glu Lys Glu Ile Asp Glu Ile Leu Asp Gln Ile Tyr Asn
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Gln Asn Ser Asn Cys Asn Asp Leu Cys Thr Ser Ala Leu Gln Phe Arg
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Leu Leu Arg Gln His Gly Phe Asn Ile Ser Pro Glu Ile Phe Ser Lys
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Phe Gln Asp Glu Asn Gly Lys Phe Lys Glu Ser Leu Ala Ser Asp Val
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Leu Gly Leu Leu Asn Leu Tyr Glu Ala Ser His Val Arg Thr His Ala
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Asp Asp Ile Leu Glu Asp Ala Leu Ala Phe Ser Thr Ile His Leu Glu
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Ser Ala Ala Pro His Leu Lys Ser Pro Leu Arg Glu Gln Val Thr His
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Ala Leu Glu Gln Cys Leu His Lys Gly Val Pro Arg Val Glu Thr Arg
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Lys Gln Glu Leu Ala Gln Val Ser Arg Trp Trp Lys Asp Leu Asp Phe
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Trp Ala Leu Gly Val Tyr Phe Glu Pro Gln Tyr Ser Gln Ala Arg Val
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Met Leu Val Lys Thr Ile Ser Met Ile Ser Ile Val Asp Asp Thr Phe
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Gln Arg Trp Asp Ile Asn Glu Ile Asp Arg Leu Pro Asp Tyr Met Lys
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Ile Ser Tyr Lys Ala Ile Leu Asp Leu Tyr Lys Asp Tyr Glu Lys Glu
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Leu Ser Ser Ala Gly Arg Ser His Ile Val Cys His Ala Ile Glu Arg
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Met Lys Glu Val Val Arg Asn Tyr Asn Val Glu Ser Thr Trp Phe Ile
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Glu Gly Tyr Met Pro Pro Val Ser Glu Tyr Leu Ser Asn Ala Leu Ala
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 Ser Ile Asp Asn Gln Val Ala Glu Lys Tyr Ala Gln Glu Ile Glu Ala
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 Tyr His Phe Glu Lys Glu Ile Asp Glu Ile Leu Asp Gln Ile Tyr Asn

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| Phe | Gln | Asp | Glu | Asn | Gly | Lys | Phe | Lys | Glu | Ser | Leu | Ala | Ser | Asp | Val | | | | | |
| | 130 | | | | | 135 | | | | | 140 | | | | | | | | | |
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| Leu | Gly | Leu | Leu | Asn | Leu | Tyr | Glu | Ala | Ser | His | Val | Arg | Thr | His | Ala | | | | | |
| 145 | | | | | 150 | | | | 155 | | | | | | 160 | | | | | |
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| Gln Arg Trp Asp Ile Asn Glu Ile Asp Arg Leu Pro Asp Tyr Met Lys | |
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| Ile Ser Tyr Lys Ala Ile Leu Asp Leu Tyr Lys Asp Tyr Glu Lys Glu | |
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| Met Lys Glu Val Val Arg Asn Tyr Asn Val Glu Ser Thr Trp Phe Ile | |
| 370 375 380 | |
| gaa gga tat atg cca cct gtt tct gaa tac cta agc aat gca cta gca | 1200 |
| Glu Gly Tyr Met Pro Val Ser Glu Tyr Leu Ser Asn Ala Leu Ala | |
| 385 390 395 400 | |
| act acc aca tat tac tac ctc gcg aca aca tcg tat ttg ggc atg aag | 1248 |
| Thr Thr Thr Tyr Tyr Tyr Leu Ala Thr Thr Ser Tyr Leu Gly Met Lys | |
| 405 410 415 | |
| tct gcc acg gag caa gat ttt gag tgg ttg tca aag aat cca aaa att | 1296 |
| Ser Ala Thr Glu Gln Asp Phe Glu Trp Leu Ser Lys Asn Pro Lys Ile | |
| 420 425 430 | |
| ctt gaa gct agt gta att ata tgt cga gtt atc gat gac aca gcc acg | 1344 |
| Leu Glu Ala Ser Val Ile Ile Cys Arg Val Ile Asp Asp Thr Ala Thr | |
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| tac gag gtt gag aaa agc agg gga caa att gca act gga att gag tgc | 1392 |
| Tyr Glu Val Glu Lys Ser Arg Gly Gln Ile Ala Thr Gly Ile Glu Cys | |
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| tgc atg aga gat tat ggt ata tca aca aaa gag gca atg gct aaa ttt | 1440 |
| Cys Met Arg Asp Tyr Gly Ile Ser Thr Lys Glu Ala Met Ala Lys Phe | |
| 465 470 475 480 | |
| caa aat atg gct gag aca gca tgg aaa gat att aat gaa gga ctt ctt | 1488 |
| Gln Asn Met Ala Glu Thr Ala Trp Lys Asp Ile Asn Glu Gly Leu Leu | |
| 485 490 495 | |
| agg ccc act ccc gtc tct aca gaa ttt tta act cct att ctc aat ctt | 1536 |
| Arg Pro Thr Pro Val Ser Thr Glu Phe Leu Thr Pro Ile Leu Asn Leu | |
| 500 505 510 | |

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gct cgt att gtt gag gtt aca tat ata cac aat cta gat gga ttc act      1584
Ala Arg Ile Val Glu Val Thr Tyr Ile His Asn Leu Asp Gly Phe Thr
      515                                520                                525

cat ccg gag aaa gtc tta aaa cct cac att att aac cta ctt gtg gac      1632
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Ser Ile Asp Asn Gln Val Ala Glu Lys Tyr Ala Gln Glu Ile Glu Ala
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Leu Lys Glu Gln Thr Arg Ser Met Leu Leu Ala Thr Gly Arg Lys Leu
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Tyr His Phe Glu Lys Glu Ile Asp Glu Ile Leu Asp Gln Ile Tyr Asn
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Gln Asn Ser Asn Cys Asn Asp Leu Cys Thr Ser Ala Leu Gln Phe Arg
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Phe Gln Asp Glu Asn Gly Lys Phe Lys Glu Ser Leu Ala Ser Asp Val
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Leu Gly Leu Leu Asn Leu Tyr Glu Ala Ser His Val Arg Thr His Ala
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Asp Asp Ile Leu Glu Asp Ala Leu Ala Phe Ser Thr Ile His Leu Glu
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Ser Ala Ala Pro His Leu Lys Ser Pro Leu Arg Glu Gln Val Thr His
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Ala Leu Glu Gln Cys Leu His Lys Gly Val Pro Arg Val Glu Thr Arg
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Phe Phe Ile Ser Ser Ile Tyr Asp Lys Glu Gln Ser Lys Asn Asn Val
      210     215     220
Leu Leu Arg Phe Ala Lys Leu Asp Phe Asn Leu Leu Gln Met Leu His
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Lys Gln Glu Leu Ala Gln Val Ser Arg Trp Trp Lys Asp Leu Asp Phe
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Val Thr Thr Leu Pro Tyr Ala Arg Asp Arg Val Val Glu Cys Tyr Phe
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 Asp Ala Tyr Gly Thr Val Lys Glu Leu Glu Ala Tyr Thr Asp Ala Ile
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 Thr Thr Thr Tyr Tyr Tyr Leu Ala Thr Thr Ser Tyr Leu Gly Met Lys
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 Ser Ala Thr Glu Gln Asp Phe Glu Trp Leu Ser Lys Asn Pro Lys Ile
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 Leu Glu Ala Ser Val Ile Ile Cys Arg Val Ile Asp Asp Thr Ala Thr
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 Tyr Glu Val Glu Lys Ser Arg Gly Gln Ile Ala Thr Gly Ile Glu Cys
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 Cys Met Arg Asp Tyr Gly Ile Ser Thr Lys Glu Ala Met Ala Lys Phe
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 Gln Asn Met Ala Glu Thr Ala Trp Lys Asp Ile Asn Glu Gly Leu Leu
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 Arg Pro Thr Pro Val Ser Thr Glu Phe Leu Thr Pro Ile Leu Asn Leu
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 Ala Arg Ile Val Glu Val Thr Tyr Ile His Asn Leu Asp Gly Phe Thr
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 Val Ala Asp Phe Ser Pro Ser Leu Trp Gly Asp Gln Phe Leu Ser Phe

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| Ser | Ile | Asp | Asn | Gln | Val | Ala | Glu | Lys | Tyr | Ala | Gln | Glu | Ile | Glu | Ala | | | | | |
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| Leu | Lys | Glu | Gln | Thr | Arg | Ser | Met | Leu | Leu | Ala | Thr | Gly | Arg | Lys | Leu | | | | | |
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| Ala | Asp | Thr | Leu | Asn | Leu | Ile | Asp | Ile | Ile | Glu | Arg | Leu | Gly | Ile | Ser | | | | | |
| | 65 | | | | 70 | | | | | 75 | | | | | 80 | | | | | |
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| Tyr | His | Phe | Glu | Lys | Glu | Ile | Asp | Glu | Ile | Leu | Asp | Gln | Ile | Tyr | Asn | | | | | |
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| caa | aac | tca | aac | tgc | aat | gat | ttg | tgc | acc | tct | gca | ctt | caa | ttt | cga | 336 | | | | |
| Gln | Asn | Ser | Asn | Cys | Asn | Asp | Leu | Cys | Thr | Ser | Ala | Leu | Gln | Phe | Arg | | | | | |
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| Phe | Gln | Asp | Glu | Asn | Gly | Lys | Phe | Lys | Glu | Ser | Leu | Ala | Ser | Asp | Val | | | | | |
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| Asp | Asp | Ile | Leu | Glu | Asp | Ala | Leu | Ala | Phe | Ser | Thr | Ile | His | Leu | Glu | | | | | |
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| ttc | ttc | atc | tca | tca | atc | tat | gac | aag | gaa | caa | tcg | aag | aat | aat | gtg | 672 | | | | |
| Phe | Phe | Ile | Ser | Ser | Ile | Tyr | Asp | Lys | Glu | Gln | Ser | Lys | Asn | Asn | Val | | | | | |
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| Leu | Leu | Arg | Phe | Ala | Lys | Leu | Asp | Phe | Asn | Leu | Leu | Gln | Met | Leu | His | | | | | |
| | 225 | | | | 230 | | | | | 235 | | | | | 240 | | | | | |

| | | | | | | | | | | | | | | | | |
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| Val | Thr | Thr | Leu | Pro | Tyr | Ala | Arg | Asp | Arg | Val | Val | Glu | Cys | Tyr | Phe | |
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| Ser | Ala | Leu | Gly | Val | Tyr | Phe | Glu | Pro | Gln | Tyr | Ser | Gln | Ala | Arg | Val | |
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| atg | ctc | gtt | aag | acc | ata | tca | atg | att | tcg | att | gtc | gat | gac | acc | ttt | 912 |
| Met | Leu | Val | Lys | Thr | Ile | Ser | Met | Ile | Ser | Ile | Val | Asp | Asp | Thr | Phe | |
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| gat | gct | tac | ggg | aca | gtt | aaa | gaa | ctt | gag | gca | tac | aca | gat | gcc | ata | 960 |
| Asp | Ala | Tyr | Gly | Thr | Val | Lys | Glu | Leu | Glu | Ala | Tyr | Thr | Asp | Ala | Ile | |
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| caa | aga | tgg | gat | atc | aac | gaa | att | gat | cgg | ctt | cct | gat | tac | atg | aaa | 1008 |
| Gln | Arg | Trp | Asp | Ile | Asn | Glu | Ile | Asp | Arg | Leu | Pro | Asp | Tyr | Met | Lys | |
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| atc | agt | tat | aaa | gct | att | cta | gat | ctc | tac | aag | gat | tat | gaa | aag | gaa | 1056 |
| Ile | Ser | Tyr | Lys | Ala | Ile | Leu | Asp | Leu | Tyr | Lys | Asp | Tyr | Glu | Lys | Glu | |
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| Leu | Ser | Ser | Ala | Gly | Arg | Ser | His | Ile | Val | Cys | His | Ala | Ile | Glu | Arg | |
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| atg | aaa | gaa | gta | gta | aga | aat | tat | aat | gtc | gag | tca | aca | tgg | ttt | att | 1152 |
| Met | Lys | Glu | Val | Val | Arg | Asn | Tyr | Asn | Val | Glu | Ser | Thr | Trp | Phe | Ile | |
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| Glu | Gly | Tyr | Met | Pro | Pro | Val | Ser | Glu | Tyr | Leu | Ser | Asn | Ala | Leu | Ala | |
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| Thr | Thr | Thr | Tyr | Tyr | Tyr | Leu | Ala | Thr | Thr | Ser | Tyr | Leu | Gly | Met | Lys | |
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| tct | gcc | acg | gag | caa | gat | ttt | gag | tgg | ttg | tca | aag | aat | cca | aaa | att | 1296 |
| Ser | Ala | Thr | Glu | Gln | Asp | Phe | Glu | Trp | Leu | Ser | Lys | Asn | Pro | Lys | Ile | |
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| ctt | gaa | gct | agt | gta | att | ata | tgg | cga | gtt | atc | gat | gac | aca | gcc | acg | 1344 |
| Leu | Glu | Ala | Ser | Val | Ile | Ile | Trp | Arg | Val | Ile | Asp | Asp | Thr | Ala | Thr | |
| | | 435 | | | | | 440 | | | | | 445 | | | | |

| | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|
| tac | gag | gtt | gag | aaa | agc | agg | gga | caa | att | gca | act | gga | att | gag | tgc | 1392 |
| Tyr | Glu | Val | Glu | Lys | Ser | Arg | Gly | Gln | Ile | Ala | Thr | Gly | Ile | Glu | Cys | |
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| Cys | Met | Arg | Asp | Tyr | Gly | Ile | Ser | Thr | Lys | Glu | Ala | Met | Ala | Lys | Phe | |
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| Gln | Asn | Met | Ala | Glu | Thr | Ala | Trp | Lys | Asp | Ile | Asn | Glu | Gly | Leu | Leu | |
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| agg | ccc | act | ccc | gtc | tct | aca | gaa | ttt | tta | act | cct | att | ctc | aat | ctt | 1536 |
| Arg | Pro | Thr | Pro | Val | Ser | Thr | Glu | Phe | Leu | Thr | Pro | Ile | Leu | Asn | Leu | |
| | | | 500 | | | | | 505 | | | | | 510 | | | |
| | | | | | | | | | | | | | | | | |
| gct | cgt | att | gtt | gag | gtt | aca | tat | ata | cac | aat | cta | gat | gga | tac | act | 1584 |
| Ala | Arg | Ile | Val | Glu | Val | Thr | Tyr | Ile | His | Asn | Leu | Asp | Gly | Tyr | Thr | |
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| His | Pro | Glu | Lys | Val | Leu | Lys | Pro | His | Ile | Ile | Asn | Leu | Leu | Val | Asp | |
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| tcc | atc | aaa | att | | | | | | | | | | | | | 1644 |
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| Val | Ala | Asp | Phe | Ser | Pro | Ser | Leu | Trp | Gly | Asp | Gln | Phe | Leu | Ser | Phe | |
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| Leu | Lys | Glu | Gln | Thr | Arg | Ser | Met | Leu | Leu | Ala | Thr | Gly | Arg | Lys | Leu | |
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| Tyr | His | Phe | Glu | Lys | Glu | Ile | Asp | Glu | Ile | Leu | Asp | Gln | Ile | Tyr | Asn | |
| | | | 85 | | | | | 90 | | | | | 95 | | | |
| Gln | Asn | Ser | Asn | Cys | Asn | Asp | Leu | Cys | Thr | Ser | Ala | Leu | Gln | Phe | Arg | |
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| Phe | Gln | Asp | Glu | Asn | Gly | Lys | Phe | Lys | Glu | Ser | Leu | Ala | Ser | Asp | Val | |
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| | | | | | | | | | | | | | | | |
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| Ser | Ala | Ala | Pro | His | Leu | Lys | Ser | Pro | Leu | Arg | Glu | Gln | Val | Thr | His |
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| Lys | Gln | Glu | Leu | Ala | Gln | Val | Ser | Arg | Trp | Trp | Lys | Asp | Leu | Asp | Phe |
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| Val | Thr | Thr | Leu | Pro | Tyr | Ala | Arg | Asp | Arg | Val | Val | Glu | Cys | Tyr | Phe |
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| Gln | Arg | Trp | Asp | Ile | Asn | Glu | Ile | Asp | Arg | Leu | Pro | Asp | Tyr | Met | Lys |
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| Thr | Thr | Thr | Tyr | Tyr | Tyr | Leu | Ala | Thr | Thr | Ser | Tyr | Leu | Gly | Met | Lys |
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| | | | 420 | | | | | 425 | | | | | 430 | | |
| Leu | Glu | Ala | Ser | Val | Ile | Ile | Trp | Arg | Val | Ile | Asp | Asp | Thr | Ala | Thr |
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| Tyr | Glu | Val | Glu | Lys | Ser | Arg | Gly | Gln | Ile | Ala | Thr | Gly | Ile | Glu | Cys |
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| Cys | Met | Arg | Asp | Tyr | Gly | Ile | Ser | Thr | Lys | Glu | Ala | Met | Ala | Lys | Phe |
| 465 | | | | | 470 | | | | | 475 | | | | | 480 |
| Gln | Asn | Met | Ala | Glu | Thr | Ala | Trp | Lys | Asp | Ile | Asn | Glu | Gly | Leu | Leu |
| | | | | 485 | | | | | 490 | | | | | 495 | |
| Arg | Pro | Thr | Pro | Val | Ser | Thr | Glu | Phe | Leu | Thr | Pro | Ile | Leu | Asn | Leu |
| | | | 500 | | | | | 505 | | | | | 510 | | |
| Ala | Arg | Ile | Val | Glu | Val | Thr | Tyr | Ile | His | Asn | Leu | Asp | Gly | Tyr | Thr |
| | | 515 | | | | | 520 | | | | | 525 | | | |
| His | Pro | Glu | Lys | Val | Leu | Lys | Pro | His | Ile | Ile | Asn | Leu | Leu | Val | Asp |
| | 530 | | | | | 535 | | | | | 540 | | | | |
| Ser | Ile | Lys | Ile | | | | | | | | | | | | |
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 Met Ala Ser Ala Ala Val Ala Asn Tyr Glu Glu Glu Ile Val Arg Pro
 1 5 10 15
 gtc gcc gac ttc tcc cct agt ctc tgg ggt gat cag ttc ctt tca ttc 96
 Val Ala Asp Phe Ser Pro Ser Leu Trp Gly Asp Gln Phe Leu Ser Phe
 20 25 30
 tcc att gat aat cag gtt gcg gaa aag tat gct caa gag att gaa gca 144
 Ser Ile Asp Asn Gln Val Ala Glu Lys Tyr Ala Gln Glu Ile Glu Ala
 35 40 45
 ttg aag gaa caa acg agg agt atg ctg tta gca acc gga agg aaa ttg 192
 Leu Lys Glu Gln Thr Arg Ser Met Leu Leu Ala Thr Gly Arg Lys Leu
 50 55 60
 gcc gat aca ttg aat ttg att gac att att gaa cgc ctt ggt ata tcc 240
 Ala Asp Thr Leu Asn Leu Ile Asp Ile Ile Glu Arg Leu Gly Ile Ser
 65 70 75 80
 tac cac ttt gag aaa gaa att gat gag att ttg gat cag att tac aac 288
 Tyr His Phe Glu Lys Glu Ile Asp Glu Ile Leu Asp Gln Ile Tyr Asn
 85 90 95
 caa aac tca aac tgc aat gat ttg tgc acc tct gca ctt caa ttt cga 336
 Gln Asn Ser Asn Cys Asn Asp Leu Cys Thr Ser Ala Leu Gln Phe Arg
 100 105 110
 ttg ctc agg caa cac ggt ttc aac atc tct cct gaa att ttc agc aaa 384
 Leu Leu Arg Gln His Gly Phe Asn Ile Ser Pro Glu Ile Phe Ser Lys
 115 120 125
 ttc caa gat gaa aat ggc aaa ttc aag gag tct ctt gct agt gat gtc 432
 Phe Gln Asp Glu Asn Gly Lys Phe Lys Glu Ser Leu Ala Ser Asp Val
 130 135 140
 tta gga tta tta aac ttg tat gaa gct tca cat gta agg act cat gct 480
 Leu Gly Leu Leu Asn Leu Tyr Glu Ala Ser His Val Arg Thr His Ala
 145 150 155 160
 gac gat atc tta gaa gac gca ctt gct ttc tcc act atc cat ctt gaa 528
 Asp Asp Ile Leu Glu Asp Ala Leu Ala Phe Ser Thr Ile His Leu Glu
 165 170 175

| | |
|---|------|
| tct gca gct cca cat ttg aaa tct cca ctt agg gag caa gtg aca cat | 576 |
| Ser Ala Ala Pro His Leu Lys Ser Pro Leu Arg Glu Gln Val Thr His | |
| 180 185 190 | |
| gcc ctt gag caa tgt ttg cac aag ggt gtt cct aga gtc gag acc cga | 624 |
| Ala Leu Glu Gln Cys Leu His Lys Gly Val Pro Arg Val Glu Thr Arg | |
| 195 200 205 | |
| ttc ttc atc tca tca atc tat gac aag gaa caa tcg aag aat aat gtg | 672 |
| Phe Phe Ile Ser Ser Ile Tyr Asp Lys Glu Gln Ser Lys Asn Asn Val | |
| 210 215 220 | |
| tta ctt cga ttt gcc aaa ttg gat ttc aac ttg ctc cag atg ttg cac | 720 |
| Leu Leu Arg Phe Ala Lys Leu Asp Phe Asn Leu Leu Gln Met Leu His | |
| 225 230 235 240 | |
| aaa caa gaa ctt gct caa gta tca agg tgg tgg aaa gat ttg gat ttt | 768 |
| Lys Gln Glu Leu Ala Gln Val Ser Arg Trp Trp Lys Asp Leu Asp Phe | |
| 245 250 255 | |
| gta aca aca ctt cca tat gct aga gat cga gta gtt gaa tgc tac ttt | 816 |
| Val Thr Thr Leu Pro Tyr Ala Arg Asp Arg Val Val Glu Cys Tyr Phe | |
| 260 265 270 | |
| tgg gca tta gga gtt tat ttt gag cct caa tac tct caa gct cgc gtc | 864 |
| Trp Ala Leu Gly Val Tyr Phe Glu Pro Gln Tyr Ser Gln Ala Arg Val | |
| 275 280 285 | |
| atg ctc gtt aag acc ata tca atg att tcg att gtc gat gac acc ttt | 912 |
| Met Leu Val Lys Thr Ile Ser Met Ile Ser Ile Val Asp Asp Thr Phe | |
| 290 295 300 | |
| gat gct tac ggt aca gtt aaa gaa ctt gag gca tac aca gat gcc ata | 960 |
| Asp Ala Tyr Gly Thr Val Lys Glu Leu Glu Ala Tyr Thr Asp Ala Ile | |
| 305 310 315 320 | |
| caa aga tgg gat atc aac gaa att gat cgg ctt cct gat tac atg aaa | 1008 |
| Gln Arg Trp Asp Ile Asn Glu Ile Asp Arg Leu Pro Asp Tyr Met Lys | |
| 325 330 335 | |
| atc agt tat aaa gct att cta gat ctc tac aag gat tat gaa aag gaa | 1056 |
| Ile Ser Tyr Lys Ala Ile Leu Asp Leu Tyr Lys Asp Tyr Glu Lys Glu | |
| 340 345 350 | |
| ttg tct agt gcc gga aga tct cat att gtc tgc cat gca ata gaa aga | 1104 |
| Leu Ser Ser Ala Gly Arg Ser His Ile Val Cys His Ala Ile Glu Arg | |
| 355 360 365 | |
| atg aaa gaa gta gta aga aat tat aat gtc gag tca aca tgg ttt att | 1152 |
| Met Lys Glu Val Val Arg Asn Tyr Asn Val Glu Ser Thr Trp Phe Ile | |
| 370 375 380 | |

gaa gga tat atg cca cct gtt tct gaa tac cta agc aat gca cta gca 1200
 Glu Gly Tyr Met Pro Pro Val Ser Glu Tyr Leu Ser Asn Ala Leu Ala
 385 390 395 400

act acc aca tat tac nns nns gcg aca aca tcg tat ttg ggc atg aag 1248
 Thr Thr Thr Tyr Tyr Xaa Xaa Ala Thr Thr Ser Tyr Leu Gly Met Lys
 405 410 415

tct gcc acg gag caa gat ttt gag tgg ttg tca aag aat cca aaa att 1296
 Ser Ala Thr Glu Gln Asp Phe Glu Trp Leu Ser Lys Asn Pro Lys Ile
 420 425 430

ctt gaa gct agt gta att ata tgt cga gtt atc gat gac aca gcc acg 1344
 Leu Glu Ala Ser Val Ile Ile Cys Arg Val Ile Asp Asp Thr Ala Thr
 435 440 445

tac gag gtt gag aaa agc agg gga caa att gca act gga att gag tgc 1392
 Tyr Glu Val Glu Lys Ser Arg Glu Gly Gln Ile Ala Thr Gly Ile Glu Cys
 450 455 460

tgc atg aga gat tat ggt ata tca aca aaa gag gca atg gct aaa ttt 1440
 Cys Met Arg Asp Tyr Gly Ile Ser Thr Lys Glu Ala Met Ala Lys Phe
 465 470 475 480

caa aat atg gct gag aca gca tgg aaa gat att aat gaa gga ctt ctt 1488
 Gln Asn Met Ala Glu Thr Ala Trp Lys Asp Ile Asn Glu Gly Leu Leu
 485 490 495

agg ccc act ccc gtc tct aca gaa ttt tta act cct att ctc aat ctt 1536
 Arg Pro Thr Pro Val Ser Thr Glu Phe Leu Thr Pro Ile Leu Asn Leu
 500 505 510

gct cgt att gtt gag gtt aca tat ata cac aat cta gat gga tac act 1584
 Ala Arg Ile Val Glu Val Thr Tyr Ile His Asn Leu Asp Gly Tyr Thr
 515 520 525

cat ccg gag aaa gtc tta aaa cct cac att att aac cta ctt gtg gac 1632
 His Pro Glu Lys Val Leu Lys Pro His Ile Ile Asn Leu Leu Val Asp
 530 535 540

tcc atc aaa att 1644
 Ser Ile Lys Ile
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| Val | Ala | Asp | Phe | Ser | Pro | Ser | Leu | Trp | Gly | Asp | Gln | Phe | Leu | Ser | Phe |
| | | | 20 | | | | | 25 | | | | | 30 | | |
| Ser | Ile | Asp | Asn | Gln | Val | Ala | Glu | Lys | Tyr | Ala | Gln | Glu | Ile | Glu | Ala |
| | | 35 | | | | | 40 | | | | | 45 | | | |
| Leu | Lys | Glu | Gln | Thr | Arg | Ser | Met | Leu | Leu | Ala | Thr | Gly | Arg | Lys | Leu |
| | 50 | | | | | 55 | | | | | 60 | | | | |
| Ala | Asp | Thr | Leu | Asn | Leu | Ile | Asp | Ile | Ile | Glu | Arg | Leu | Gly | Ile | Ser |
| 65 | | | | 70 | | | | | | 75 | | | | | 80 |
| Tyr | His | Phe | Glu | Lys | Glu | Ile | Asp | Glu | Ile | Leu | Asp | Gln | Ile | Tyr | Asn |
| | | | 85 | | | | | 90 | | | | | | 95 | |
| Gln | Asn | Ser | Asn | Cys | Asn | Asp | Leu | Cys | Thr | Ser | Ala | Leu | Gln | Phe | Arg |
| | | | 100 | | | | | 105 | | | | | 110 | | |
| Leu | Leu | Arg | Gln | His | Gly | Phe | Asn | Ile | Ser | Pro | Glu | Ile | Phe | Ser | Lys |
| | | 115 | | | | | 120 | | | | | 125 | | | |
| Phe | Gln | Asp | Glu | Asn | Gly | Lys | Phe | Lys | Glu | Ser | Leu | Ala | Ser | Asp | Val |
| | 130 | | | | | 135 | | | | | 140 | | | | |
| Leu | Gly | Leu | Leu | Asn | Leu | Tyr | Glu | Ala | Ser | His | Val | Arg | Thr | His | Ala |
| 145 | | | | 150 | | | | | | 155 | | | | | 160 |
| Asp | Asp | Ile | Leu | Glu | Asp | Ala | Leu | Ala | Phe | Ser | Thr | Ile | His | Leu | Glu |
| | | | 165 | | | | | | 170 | | | | | 175 | |
| Ser | Ala | Ala | Pro | His | Leu | Lys | Ser | Pro | Leu | Arg | Glu | Gln | Val | Thr | His |
| | | | 180 | | | | | 185 | | | | | 190 | | |
| Ala | Leu | Glu | Gln | Cys | Leu | His | Lys | Gly | Val | Pro | Arg | Val | Glu | Thr | Arg |
| | | 195 | | | | | 200 | | | | | 205 | | | |
| Phe | Phe | Ile | Ser | Ser | Ile | Tyr | Asp | Lys | Glu | Gln | Ser | Lys | Asn | Asn | Val |
| | 210 | | | | | 215 | | | | | 220 | | | | |
| Leu | Leu | Arg | Phe | Ala | Lys | Leu | Asp | Phe | Asn | Leu | Leu | Gln | Met | Leu | His |
| 225 | | | | | 230 | | | | | 235 | | | | | 240 |
| Lys | Gln | Glu | Leu | Ala | Gln | Val | Ser | Arg | Trp | Trp | Lys | Asp | Leu | Asp | Phe |
| | | | 245 | | | | | | 250 | | | | 255 | | |
| Val | Thr | Thr | Leu | Pro | Tyr | Ala | Arg | Asp | Arg | Val | Val | Glu | Cys | Tyr | Phe |
| | | | 260 | | | | | 265 | | | | | 270 | | |
| Trp | Ala | Leu | Gly | Val | Tyr | Phe | Glu | Pro | Gln | Tyr | Ser | Gln | Ala | Arg | Val |
| | 275 | | | | | | 280 | | | | | 285 | | | |
| Met | Leu | Val | Lys | Thr | Ile | Ser | Met | Ile | Ser | Ile | Val | Asp | Asp | Thr | Phe |
| | 290 | | | | | 295 | | | | | 300 | | | | |
| Asp | Ala | Tyr | Gly | Thr | Val | Lys | Glu | Leu | Glu | Ala | Tyr | Thr | Asp | Ala | Ile |
| 305 | | | | | 310 | | | | | 315 | | | | | 320 |
| Gln | Arg | Trp | Asp | Ile | Asn | Glu | Ile | Asp | Arg | Leu | Pro | Asp | Tyr | Met | Lys |
| | | | 325 | | | | | | 330 | | | | | 335 | |
| Ile | Ser | Tyr | Lys | Ala | Ile | Leu | Asp | Leu | Tyr | Lys | Asp | Tyr | Glu | Lys | Glu |
| | | | 340 | | | | | 345 | | | | | 350 | | |
| Leu | Ser | Ser | Ala | Gly | Arg | Ser | His | Ile | Val | Cys | His | Ala | Ile | Glu | Arg |
| | | 355 | | | | | 360 | | | | | 365 | | | |
| Met | Lys | Glu | Val | Val | Arg | Asn | Tyr | Asn | Val | Glu | Ser | Thr | Trp | Phe | Ile |
| | 370 | | | | | 375 | | | | | 380 | | | | |
| Glu | Gly | Tyr | Met | Pro | Pro | Val | Ser | Glu | Tyr | Leu | Ser | Asn | Ala | Leu | Ala |
| 385 | | | | | 390 | | | | | 395 | | | | | 400 |
| Thr | Thr | Thr | Tyr | Tyr | Xaa | Xaa | Ala | Thr | Thr | Ser | Tyr | Leu | Gly | Met | Lys |
| | | | 405 | | | | | | 410 | | | | | 415 | |
| Ser | Ala | Thr | Glu | Gln | Asp | Phe | Glu | Trp | Leu | Ser | Lys | Asn | Pro | Lys | Ile |
| | | | 420 | | | | | 425 | | | | | 430 | | |
| Leu | Glu | Ala | Ser | Val | Ile | Ile | Cys | Arg | Val | Ile | Asp | Asp | Thr | Ala | Thr |

[illegible]

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<223> primer
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<212> DNA
<213> Artificial Sequence
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<223> primer
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<210> 16

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 <220>
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 <210> 17
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 <212> DNA
 <213> Artificial Sequence

 <220>
 <223> primer

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 <220>
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 <212> DNA
 <213> Abies grandis

 <220>
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 <222> (6)...(1892)
 <223> pinene synthase

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 cac aaa tcg ttg atc agt tct acc cat gag ctt aag gct ctc tct aga 98
 His Lys Ser Leu Ile Ser Ser Thr His Glu Leu Lys Ala Leu Ser Arg
 20 25 30

| | |
|---|-----|
| aca att cca gct cta gga atg agt agg cga ggg aaa tct atc act cct | 146 |
| Thr Ile Pro Ala Leu Gly Met Ser Arg Arg Gly Lys Ser Ile Thr Pro | |
| 35 40 45 | |
| tcc atc agc atg agc tct acc acc gtt gta acc gat gat ggt gta cga | 194 |
| Ser Ile Ser Met Ser Ser Thr Thr Val Val Thr Asp Asp Gly Val Arg | |
| 50 55 60 | |
| aga cgc atg ggc gat ttc cat tcc aac ctc tgg gac gat gat gtc ata | 242 |
| Arg Arg Met Gly Asp Phe His Ser Asn Leu Trp Asp Asp Val Ile | |
| 65 70 75 | |
| cag tct tta cca acg gct tat gag gaa aaa tcg tac ctg gag cgt gct | 290 |
| Gln Ser Leu Pro Thr Ala Tyr Glu Glu Lys Ser Tyr Leu Glu Arg Ala | |
| 80 85 90 95 | |
| gag aaa ctg atc ggg gaa gta aag aac atg ttc aat tcg atg tca tta | 338 |
| Glu Lys Leu Ile Gly Glu Val Lys Asn Met Phe Asn Ser Met Ser Leu | |
| 100 105 110 | |
| gaa gat gga gag tta atg agt ccg ctc aat gat ctc att caa cgc ctt | 386 |
| Glu Asp Gly Glu Leu Met Ser Pro Leu Asn Asp Leu Ile Gln Arg Leu | |
| 115 120 125 | |
| tgg att gtc gac agc ctt gaa cgt ttg ggg atc cat aga cat ttc aaa | 434 |
| Trp Ile Val Asp Ser Leu Glu Arg Leu Gly Ile His Arg His Phe Lys | |
| 130 135 140 | |
| gat gag ata aaa tcg gcg ctt gat tat gtt tac agt tat tgg ggc gaa | 482 |
| Asp Glu Ile Lys Ser Ala Leu Asp Tyr Val Tyr Ser Tyr Trp Gly Glu | |
| 145 150 155 | |
| aat ggc atc gga tgc ggg agg gag agt gtt gtt act gat ctg aac tca | 530 |
| Asn Gly Ile Gly Cys Gly Arg Glu Ser Val Val Thr Asp Leu Asn Ser | |
| 160 165 170 175 | |
| act gcg ttg ggg ctt cga acc cta cga cta cac gga tac ccg gtg tct | 578 |
| Thr Ala Leu Gly Leu Arg Thr Leu Arg Leu His Gly Tyr Pro Val Ser | |
| 180 185 190 | |
| tca gat gtt ttc aaa gct ttc aaa ggc caa aat ggg cag ttt tcc tgc | 626 |
| Ser Asp Val Phe Lys Ala Phe Lys Gly Gln Asn Gly Gln Phe Ser Cys | |
| 195 200 205 | |
| tct gaa aat att cag aca gat gaa gag atc aga ggc gtt ctg aat tta | 674 |
| Ser Glu Asn Ile Gln Thr Asp Glu Glu Ile Arg Gly Val Leu Asn Leu | |
| 210 215 220 | |
| ttc cgg gcc tcc ctc att gcc ttt cca ggg gag aaa att atg gat gag | 722 |
| Phe Arg Ala Ser Leu Ile Ala Phe Pro Gly Glu Lys Ile Met Asp Glu | |
| 225 230 235 | |

| | |
|---|------|
| gct gaa atc ttc tct acc aaa tat tta aaa gaa gcc ctg caa aag att | 770 |
| Ala Glu Ile Phe Ser Thr Lys Tyr Leu Lys Glu Ala Leu Gln Lys Ile | |
| 240 245 250 255 | |
| ccg gtc tcc agt ctt tcg cga gag atc ggg gac gtt ttg gaa tat ggt | 818 |
| Pro Val Ser Ser Leu Ser Arg Glu Ile Gly Asp Val Leu Glu Tyr Gly | |
| 260 265 270 | |
| tgg cac aca tat ttg ccg cga ttg gaa gca agg aat tac atc caa gtc | 866 |
| Trp His Thr Tyr Leu Pro Arg Leu Glu Ala Arg Asn Tyr Ile Gln Val | |
| 275 280 285 | |
| ttt gga cag gac act gag aac acg aag tca tat gtg aag agc aaa aaa | 914 |
| Phe Gly Gln Asp Thr Glu Asn Thr Lys Ser Tyr Val Lys Ser Lys Lys | |
| 290 295 300 | |
| ctt tta gaa ctc gca aaa ttg gag ttc aac atc ttt caa tcc tta caa | 962 |
| Leu Leu Glu Leu Ala Lys Leu Glu Phe Asn Ile Phe Gln Ser Leu Gln | |
| 305 310 315 | |
| aag agg gag tta gaa agt ctg gtc aga tgg tgg aaa gaa tcg ggt ttt | 1010 |
| Lys Arg Glu Leu Glu Ser Leu Val Arg Trp Trp Lys Glu Ser Gly Phe | |
| 320 325 330 335 | |
| cct gag atg acc ttc tgc cga cat cgt cac gtg gaa tac tac act ttg | 1058 |
| Pro Glu Met Thr Phe Cys Arg His Arg His Val Glu Tyr Tyr Thr Leu | |
| 340 345 350 | |
| gct tcc tgc att gcg ttc gag cct caa cat tct gga ttc aga ctc ggc | 1106 |
| Ala Ser Cys Ile Ala Phe Glu Pro Gln His Ser Gly Phe Arg Leu Gly | |
| 355 360 365 | |
| ttt gcc aag acg tgt cat ctt atc acg gtt ctt gac gat atg tac gac | 1154 |
| Phe Ala Lys Thr Cys His Leu Ile Thr Val Leu Asp Asp Met Tyr Asp | |
| 370 375 380 | |
| acc ttc ggc aca gta gac gag ctg gaa ctc ttc aca gcg aca atg aag | 1202 |
| Thr Phe Gly Thr Val Asp Glu Leu Glu Leu Phe Thr Ala Thr Met Lys | |
| 385 390 395 | |
| aga tgg gat ccg tcc tcg ata gat tgc ctt cca gaa tat atg aaa gga | 1250 |
| Arg Trp Asp Pro Ser Ser Ile Asp Cys Leu Pro Glu Tyr Met Lys Gly | |
| 400 405 410 415 | |
| gtg tac ata gcg gtt tac gac acc gta aat gaa atg gct cga gag gca | 1298 |
| Val Tyr Ile Ala Val Tyr Asp Thr Val Asn Glu Met Ala Arg Glu Ala | |
| 420 425 430 | |
| gag gag gct caa ggc cga gat acg ctc aca tat gct cgg gaa gct tgg | 1346 |
| Glu Glu Ala Gln Gly Arg Asp Thr Leu Thr Tyr Ala Arg Glu Ala Trp | |
| 435 440 445 | |
| gag gct tat att gat tcg tat atg caa gaa gca agg tgg atc gcc act | 1394 |

| | | | | | | | | | | | | | | | | | |
|------------|------------|------------|------------|------------|------------|------------|------------|------------|-----|-----|-----|-----|-----|-----|-----|------|--|
| Glu | Ala | Tyr | Ile | Asp | Ser | Tyr | Met | Gln | Glu | Ala | Arg | Trp | Ile | Ala | Thr | | |
| | 450 | | | | | | 455 | | | | | 460 | | | | | |
| ggt | tac | ctg | ccc | tcc | ttt | gat | gag | tac | tac | gag | aat | ggg | aaa | gtt | agc | 1442 | |
| Gly | Tyr | Leu | Pro | Ser | Phe | Asp | Glu | Tyr | Tyr | Glu | Asn | Gly | Lys | Val | Ser | | |
| | 465 | | | | | 470 | | | | | 475 | | | | | | |
| tgt | ggt | cat | cgc | ata | tcc | gca | ttg | caa | ccc | att | ctg | aca | atg | gac | atc | 1490 | |
| Cys | Gly | His | Arg | Ile | Ser | Ala | Leu | Gln | Pro | Ile | Leu | Thr | Met | Asp | Ile | | |
| 480 | | | | | 485 | | | | | 490 | | | | | 495 | | |
| ccc | ttt | cct | gat | cat | atc | ctc | aag | gaa | gtt | gac | ttc | cca | tca | aag | ctt | 1538 | |
| Pro | Phe | Pro | Asp | His | Ile | Leu | Lys | Glu | Val | Asp | Phe | Pro | Ser | Lys | Leu | | |
| | | | | 500 | | | | | 505 | | | | | 510 | | | |
| aac | gac | ttg | gca | tgt | gcc | atc | ctt | cga | tta | cga | ggg | gat | acg | cgg | tgc | 1586 | |
| Asn | Asp | Leu | Ala | Cys | Ala | Ile | Leu | Arg | Leu | Arg | Gly | Asp | Thr | Arg | Cys | | |
| | | | 515 | | | | | 520 | | | | | 525 | | | | |
| tac | aag | gcg | gac | agg | gct | cgt | gga | gaa | gaa | gct | tcc | tct | ata | tca | tgt | 1634 | |
| Tyr | Lys | Ala | Asp | Arg | Ala | Arg | Gly | Glu | Glu | Ala | Ser | Ser | Ile | Ser | Cys | | |
| | | 530 | | | | | 535 | | | | | 540 | | | | | |
| tat | atg | aaa | gac | aat | cct | gga | gta | tca | gag | gaa | gat | gct | ctc | gat | cat | 1682 | |
| Tyr | Met | Lys | Asp | Asn | Pro | Gly | Val | Ser | Glu | Glu | Asp | Ala | Leu | Asp | His | | |
| | 545 | | | | | 550 | | | | | 555 | | | | | | |
| atc | aac | gcc | atg | atc | agt | gac | gta | atc | aaa | gga | tta | aat | tgg | gaa | ctt | 1730 | |
| Ile | Asn | Ala | Met | Ile | Ser | Asp | Val | Ile | Lys | Gly | Leu | Asn | Trp | Glu | Leu | | |
| 560 | | | | | 565 | | | | | 570 | | | | | 575 | | |
| ctc | aaa | cca | gac | atc | aat | gtt | ccc | atc | tgc | gcg | aag | aaa | cat | gct | ttt | 1778 | |
| Leu | Lys | Pro | Asp | Ile | Asn | Val | Pro | Ile | Ser | Ala | Lys | Lys | His | Ala | Phe | | |
| | | | | 580 | | | | | 585 | | | | | 590 | | | |
| gac | atc | gcc | aga | gct | ttc | cat | tac | ggc | tac | aaa | tac | cga | gac | ggc | tac | 1826 | |
| Asp | Ile | Ala | Arg | Ala | Phe | His | Tyr | Gly | Tyr | Lys | Tyr | Arg | Asp | Gly | Tyr | | |
| | | | 595 | | | | | 600 | | | | | 605 | | | | |
| agc | gtt | gcc | aac | gtt | gaa | acg | aag | agt | ttg | gtc | acg | aga | acc | ctc | ctt | 1874 | |
| Ser | Val | Ala | Asn | Val | Glu | Thr | Lys | Ser | Leu | Val | Thr | Arg | Thr | Leu | Leu | | |
| | | 610 | | | | | 615 | | | | | 620 | | | | | |
| gaa | tct | gtg | cct | ttg | tag | caacagctca | aatctatgcc | ctatgctatg | | | | | | | | 1922 | |
| Glu | Ser | Val | Pro | Leu | * | | | | | | | | | | | | |
| | 625 | | | | | | | | | | | | | | | | |
| tcgggttaaa | atatatgtgg | aaggtagccg | ttggatgtag | aggataagtt | tggtataatt | | | | | | | | | | | 1982 | |
| taataaagtt | gtaattttaa | aaaaaaaaaa | aaaaaa | | | | | | | | | | | | | 2018 | |

<210> 20
 <211> 628
 <212> PRT

<213> Abies grandis

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<400> 20
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Lys Ser Leu Ile Ser Ser Thr His Glu Leu Lys Ala Leu Ser Arg Thr
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Ile Pro Ala Leu Gly Met Ser Arg Arg Gly Lys Ser Ile Thr Pro Ser
 35      40      45
Ile Ser Met Ser Ser Thr Thr Val Val Thr Asp Asp Gly Val Arg Arg
 50      55      60
Arg Met Gly Asp Phe His Ser Asn Leu Trp Asp Asp Val Ile Gln
 65      70      75      80
Ser Leu Pro Thr Ala Tyr Glu Glu Lys Ser Tyr Leu Glu Arg Ala Glu
 85      90      95
Lys Leu Ile Gly Glu Val Lys Asn Met Phe Asn Ser Met Ser Leu Glu
 100     105     110
Asp Gly Glu Leu Met Ser Pro Leu Asn Asp Leu Ile Gln Arg Leu Trp
 115     120     125
Ile Val Asp Ser Leu Glu Arg Leu Gly Ile His Arg His Phe Lys Asp
 130     135     140
Glu Ile Lys Ser Ala Leu Asp Tyr Val Tyr Ser Tyr Trp Gly Glu Asn
 145     150     155     160
Gly Ile Gly Cys Gly Arg Glu Ser Val Val Thr Asp Leu Asn Ser Thr
 165     170     175
Ala Leu Gly Leu Arg Thr Leu Arg Leu His Gly Tyr Pro Val Ser Ser
 180     185     190
Asp Val Phe Lys Ala Phe Lys Gly Gln Asn Gly Gln Phe Ser Cys Ser
 195     200     205
Glu Asn Ile Gln Thr Asp Glu Glu Ile Arg Gly Val Leu Asn Leu Phe
 210     215     220
Arg Ala Ser Leu Ile Ala Phe Pro Gly Glu Lys Ile Met Asp Glu Ala
 225     230     235     240
Glu Ile Phe Ser Thr Lys Tyr Leu Lys Glu Ala Leu Gln Lys Ile Pro
 245     250     255
Val Ser Ser Leu Ser Arg Glu Ile Gly Asp Val Leu Glu Tyr Gly Trp
 260     265     270
His Thr Tyr Leu Pro Arg Leu Glu Ala Arg Asn Tyr Ile Gln Val Phe
 275     280     285
Gly Gln Asp Thr Glu Asn Thr Lys Ser Tyr Val Lys Ser Lys Lys Leu
 290     295     300
Leu Glu Leu Ala Lys Leu Glu Phe Asn Ile Phe Gln Ser Leu Gln Lys
 305     310     315     320
Arg Glu Leu Glu Ser Leu Val Arg Trp Trp Lys Glu Ser Gly Phe Pro
 325     330     335
Glu Met Thr Phe Cys Arg His Arg His Val Glu Tyr Tyr Thr Leu Ala
 340     345     350
Ser Cys Ile Ala Phe Glu Pro Gln His Ser Gly Phe Arg Leu Gly Phe
 355     360     365
Ala Lys Thr Cys His Leu Ile Thr Val Leu Asp Asp Met Tyr Asp Thr
 370     375     380
Phe Gly Thr Val Asp Glu Leu Glu Leu Phe Thr Ala Thr Met Lys Arg
 385     390     395     400

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Trp Asp Pro Ser Ser Ile Asp Cys Leu Pro Glu Tyr Met Lys Gly Val
 405 410 415
 Tyr Ile Ala Val Tyr Asp Thr Val Asn Glu Met Ala Arg Glu Ala Glu
 420 425 430
 Glu Ala Gln Gly Arg Asp Thr Leu Thr Tyr Ala Arg Glu Ala Trp Glu
 435 440 445
 Ala Tyr Ile Asp Ser Tyr Met Gln Glu Ala Arg Trp Ile Ala Thr Gly
 450 455 460
 Tyr Leu Pro Ser Phe Asp Glu Tyr Tyr Glu Asn Gly Lys Val Ser Cys
 465 470 475 480
 Gly His Arg Ile Ser Ala Leu Gln Pro Ile Leu Thr Met Asp Ile Pro
 485 490 495
 Phe Pro Asp His Ile Leu Lys Glu Val Asp Phe Pro Ser Lys Leu Asn
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 Asp Leu Ala Cys Ala Ile Leu Arg Leu Arg Gly Asp Thr Arg Cys Tyr
 515 520 525
 Lys Ala Asp Arg Ala Arg Gly Glu Glu Ala Ser Ser Ile Ser Cys Tyr
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 Met Lys Asp Asn Pro Gly Val Ser Glu Glu Asp Ala Leu Asp His Ile
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 Asn Ala Met Ile Ser Asp Val Ile Lys Gly Leu Asn Trp Glu Leu Leu
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 Lys Pro Asp Ile Asn Val Pro Ile Ser Ala Lys Lys His Ala Phe Asp
 580 585 590
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 Ser Val Pro Leu
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<210> 21

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<212> DNA

<213> *Mentha spicata*

<220>

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<222> (29)...(1828)

<223> 4S-limonene synthase

<400> 21

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 Met Ala Leu Lys Val Leu Ser Val
 1 5

 gca act caa atg gcg att cct agc aac cta acg aca tgt ctt caa ccc 100
 Ala Thr Gln Met Ala Ile Pro Ser Asn Leu Thr Thr Cys Leu Gln Pro
 10 15 20

 tca cac ttc aaa tct tct cca aaa ctg tta tct agc act aac agt agt 148
 Ser His Phe Lys Ser Ser Pro Lys Leu Leu Ser Ser Thr Asn Ser Ser
 25 30 35 40

| | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| agt | cgg | tct | cgc | ctc | cgt | gtg | tat | tgc | tcc | tcc | tcg | caa | ctc | act | act | 196 |
| Ser | Arg | Ser | Arg | Leu | Arg | Val | Tyr | Cys | Ser | Ser | Ser | Gln | Leu | Thr | Thr | |
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| gaa | aga | cga | tcc | gga | aac | tac | aac | cct | tct | cgt | tgg | gat | gtc | aac | ttc | 244 |
| Glu | Arg | Arg | Ser | Gly | Asn | Tyr | Asn | Pro | Ser | Arg | Trp | Asp | Val | Asn | Phe | |
| | | | 60 | | | | | 65 | | | | | 70 | | | |
| atc | caa | tcg | ctt | ctc | agt | gac | tat | aag | gag | gac | aaa | cac | gtg | att | agg | 292 |
| Ile | Gln | | Leu | Leu | Ser | Asp | Tyr | Lys | Glu | Asp | Lys | His | Val | Ile | Arg | |
| | | 75 | | | | | 80 | | | | 85 | | | | | |
| gct | tct | gag | ctg | gtc | act | ttg | gtg | aag | atg | gaa | ctg | gag | aaa | gaa | acg | 340 |
| Ala | Ser | Glu | Leu | Val | Thr | Leu | Val | Lys | Met | Glu | Leu | Glu | Lys | Glu | Thr | |
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| gat | caa | att | cga | caa | ctt | gag | ttg | atc | gat | gac | ttg | cag | agg | atg | ggg | 388 |
| Asp | Gln | Ile | Arg | Gln | Leu | Glu | Leu | Ile | Asp | Asp | Leu | Gln | Arg | Met | Gly | |
| 105 | | | | 110 | | | | | | 115 | | | | | 120 | |
| ctg | tcc | gat | cat | ttc | caa | aat | gag | ttc | aaa | gaa | atc | ttg | tcc | tct | ata | 436 |
| Leu | Ser | Asp | His | Phe | Gln | Asn | Glu | Phe | Lys | Glu | Ile | Leu | Ser | Ser | Ile | |
| | | | | 125 | | | | 130 | | | | | | 135 | | |
| tat | ctc | gac | cat | cac | tat | tac | aag | aac | cct | ttt | cca | aaa | gaa | gaa | agg | 484 |
| Tyr | Leu | Asp | His | His | Tyr | Tyr | Lys | Asn | Pro | Phe | Pro | Lys | Glu | Glu | Arg | |
| | | | 140 | | | | 145 | | | | | | 150 | | | |
| gat | ctc | tac | tcc | aca | tct | ctt | gca | ttt | agg | ctc | ctc | aga | gaa | cat | ggt | 532 |
| Asp | Leu | Tyr | Ser | Thr | Ser | Leu | Ala | Phe | Arg | Leu | Leu | Arg | Glu | His | Gly | |
| | | 155 | | | | | 160 | | | | | 165 | | | | |
| ttt | caa | gtc | gca | caa | gag | gta | ttc | gat | agt | ttc | aag | aac | gag | gag | ggt | 580 |
| Phe | Gln | Val | Ala | Gln | Glu | Val | Phe | Asp | Ser | Phe | Lys | Asn | Glu | Glu | Gly | |
| | 170 | | | | 175 | | | | | | 180 | | | | | |
| gag | ttc | aaa | gaa | agc | ctt | agc | gac | gac | acc | aga | gga | ttg | ttg | caa | ctg | 628 |
| Glu | Phe | Lys | Glu | Ser | Leu | Ser | Asp | Asp | Thr | Arg | Gly | Leu | Leu | Gln | Leu | |
| 185 | | | | | 190 | | | | | 195 | | | | | 200 | |
| tat | gaa | gct | tcc | ttt | ctg | ttg | acg | gaa | ggc | gaa | acc | acg | ctc | gag | tca | 676 |
| Tyr | Glu | Ala | Ser | Phe | Leu | Leu | Thr | Glu | Gly | Glu | Thr | Thr | Leu | Glu | Ser | |
| | | | | 205 | | | | | 210 | | | | | 215 | | |
| gcg | agg | gaa | ttc | gcc | acc | aaa | ttt | ttg | gag | gaa | aaa | gtg | aac | gag | ggt | 724 |
| Ala | Arg | Glu | Phe | Ala | Thr | Lys | Phe | Leu | Glu | Glu | Lys | Val | Asn | Glu | Gly | |
| | | | 220 | | | | | 225 | | | | | 230 | | | |
| ggt | gtt | gat | ggc | gac | ctt | tta | aca | aga | atc | gca | tat | tct | ttg | gac | atc | 772 |
| Gly | Val | Asp | Gly | Asp | Leu | Leu | Thr | Arg | Ile | Ala | Tyr | Ser | Leu | Asp | Ile | |
| | | 235 | | | | | 240 | | | | | 245 | | | | |

| | |
|---|------|
| cct ctt cat tgg agg att aaa agg cca aat gca cct gtg tgg atc gaa Pro Leu His Trp Arg Ile Lys Arg Pro Asn Ala Pro Val Trp Ile Glu 250 255 260 | 820 |
| tgg tat agg aag agg ccc gac atg aat cca gta gtg ttg gag ctt gcc Trp Tyr Arg Lys Arg Pro Asp Met Asn Pro Val Val Leu Glu Leu Ala 265 270 275 280 | 868 |
| ata ctc gac tta aat att gtt caa gca caa ttt caa gaa gag ctc aaa Ile Leu Asp Leu Asn Ile Val Gln Ala Gln Phe Gln Glu Glu Leu Lys 285 290 295 | 916 |
| gaa tcc ttc agg tgg tgg aga aat act ggg ttt gtt gag aag ctg ccc Glu Ser Phe Arg Trp Trp Arg Asn Thr Gly Phe Val Glu Lys Leu Pro 300 305 310 | 964 |
| ttc gca agg gat aga ctg gtg gaa tgc tac ttt tgg aat act ggg atc Phe Ala Arg Asp Arg Leu Val Glu Cys Tyr Phe Trp Asn Thr Gly Ile 315 320 325 | 1012 |
| atc gag cca cgt cag cat gca agt gca agg ata atg atg ggc aaa gtc Ile Glu Pro Arg Gln His Ala Ser Ala Arg Ile Met Met Gly Lys Val 330 335 340 | 1060 |
| aac gct ctg att acg gtg atc gat gat att tat gat gtc tat ggc acc Asn Ala Leu Ile Thr Val Ile Asp Asp Ile Tyr Asp Val Tyr Gly Thr 345 350 355 360 | 1108 |
| tta gaa gaa ctc gaa caa ttc act gac ctc att cga aga tgg gat ata Leu Glu Glu Leu Glu Gln Phe Thr Asp Leu Ile Arg Arg Trp Asp Ile 365 370 375 | 1156 |
| aac tca atc gac caa ctt ccc gat tac atg caa ctg tgc ttt ctt gca Asn Ser Ile Asp Gln Leu Pro Asp Tyr Met Gln Leu Cys Phe Leu Ala 380 385 390 | 1204 |
| ctc aac aac ttc gtc gat gat aca tcg tac gat gtt atg aag gag aaa Leu Asn Asn Phe Val Asp Asp Thr Ser Tyr Asp Val Met Lys Glu Lys 395 400 405 | 1252 |
| ggc gtc aac gtt ata ccc tac ctg cgg caa tcg tgg gtt gat ttg gcg Gly Val Asn Val Ile Pro Tyr Leu Arg Gln Ser Trp Val Asp Leu Ala 410 415 420 | 1300 |
| gat aag tat atg gta gag gca cgg tgg ttc tac ggc ggg cac aaa cca Asp Lys Tyr Met Val Glu Ala Arg Trp Phe Tyr Gly Gly His Lys Pro 425 430 435 440 | 1348 |
| agt ttg gaa gag tat ttg gag aac tca tgg cag tcg ata agt ggg ccc Ser Leu Glu Glu Tyr Leu Glu Asn Ser Trp Gln Ser Ile Ser Gly Pro 445 450 455 | 1396 |
| tgt atg tta acg cac ata ttc ttc cga gta aca gat tcg ttc aca aag | 1444 |

| | | | | | | | | | | | | | | | | |
|------------|------------|------------|-------------|-------------|------------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|
| Cys | Met | Leu | Thr | His | Ile | Phe | Phe | Arg | Val | Thr | Asp | Ser | Phe | Thr | Lys | |
| | | | 460 | | | | | 465 | | | | | 470 | | | |
| gag | acc | gtc | gac | agt | ttg | tac | aaa | tac | cac | gat | tta | gtt | cgt | tgg | tca | 1492 |
| Glu | Thr | Val | Asp | Ser | Leu | Tyr | Lys | Tyr | His | Asp | Leu | Val | Arg | Trp | Ser | |
| | | 475 | | | | | 480 | | | | | 485 | | | | |
| tcc | ttc | gtt | ctg | cgg | ctt | gct | gat | gat | ttg | gga | acc | tcg | gtg | gaa | gag | 1540 |
| Ser | Phe | Val | Leu | Arg | Leu | Ala | Asp | Asp | Leu | Gly | Thr | Ser | Val | Glu | Glu | |
| | 490 | | | | | 495 | | | | | 500 | | | | | |
| gtg | agc | aga | ggg | gat | gtg | ccg | aaa | tca | ctt | cag | tgc | tac | atg | agt | gac | 1588 |
| Val | Ser | Arg | Gly | Asp | Val | Pro | Lys | Ser | Leu | Gln | Cys | Tyr | Met | Ser | Asp | |
| 505 | | | | | 510 | | | | | 515 | | | | | 520 | |
| tac | aat | gca | tcg | gag | gcg | gag | gcg | cgg | aag | cac | gtg | aaa | tgg | ctg | ata | 1636 |
| Tyr | Asn | Ala | Ser | Glu | Ala | Glu | Ala | Arg | Lys | His | Val | Lys | Trp | Leu | Ile | |
| | | | | 525 | | | | | 530 | | | | | 535 | | |
| gcg | gag | gtg | tgg | aag | aag | atg | aat | gcg | gag | agg | gtg | tcg | aag | gat | tct | 1684 |
| Ala | Glu | Val | Trp | Lys | Lys | Met | Asn | Ala | Glu | Arg | Val | Ser | Lys | Asp | Ser | |
| | | | 540 | | | | | 545 | | | | | 550 | | | |
| cca | ttc | ggc | aaa | gat | ttt | ata | gga | tgt | gca | gtt | gat | tta | gga | agg | atg | 1732 |
| Pro | Phe | Gly | Lys | Asp | Phe | Ile | Gly | Cys | Ala | Val | Asp | Leu | Gly | Arg | Met | |
| | | 555 | | | | | 560 | | | | | 565 | | | | |
| gcg | cag | ttg | atg | tac | cat | aat | gga | gat | ggg | cac | ggc | aca | caa | cac | cct | 1780 |
| Ala | Gln | Leu | Met | Tyr | His | Asn | Gly | Asp | Gly | His | Gly | Thr | Gln | His | Pro | |
| | 570 | | | | | 575 | | | | | 580 | | | | | |
| att | ata | cat | caa | caa | atg | acc | aga | acc | tta | ttc | gag | ccc | ttt | gca | tga | 1828 |
| Ile | Ile | His | Gln | Gln | Met | Thr | Arg | Thr | Leu | Phe | Glu | Pro | Phe | Ala | * | |
| 585 | | | | | 590 | | | | | 595 | | | | | | |
| gagatgatga | cgagccatcg | tttacttact | ttaaattctac | caaagttttt | cgaaggcata | 1888 | | | | | | | | | | |
| gttcgtaatt | tttcaagcac | caataaataa | ggagaatcgg | ctcaaacaaa | cgtggcattt | 1948 | | | | | | | | | | |
| gccaccacgt | gagcacaagg | gagagtctgt | cgctcgtttat | ggatgaacta | ttcaattttt | 2008 | | | | | | | | | | |
| atgcatgtaa | taattaagtt | caagttcaag | agccttctgc | atattttaact | atgtatttga | 2068 | | | | | | | | | | |
| atttatcgag | tgtgattttc | tgtctttggc | aacatatatt | tttgtcatat | gtggcatctt | 2128 | | | | | | | | | | |
| attatgatat | catacagtgt | ttatggatga | tatgatacta | tc | | 2170 | | | | | | | | | | |

<210> 22

<211> 599

<212> PRT

<213> *Mentha spicata*

<400> 22

| | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|--|
| Met | Ala | Leu | Lys | Val | Leu | Ser | Val | Ala | Thr | Gln | Met | Ala | Ile | Pro | Ser | |
| 1 | | | 5 | | | | | 10 | | | | | 15 | | | |
| Asn | Leu | Thr | Thr | Cys | Leu | Gln | Pro | Ser | His | Phe | Lys | Ser | Ser | Pro | Lys | |
| | | | 20 | | | | | 25 | | | | | 30 | | | |
| Leu | Leu | Ser | Ser | Thr | Asn | Ser | Ser | Ser | Arg | Ser | Arg | Leu | Arg | Val | Tyr | |

| | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| | | | | | | | | | | | | | | | |
| Cys | Ser | Ser | Ser | Gln | Leu | Thr | Thr | Glu | Arg | Arg | Ser | Gly | Asn | Tyr | Asn |
| Pro | 50 | | | | | 55 | | | | | 60 | | | | |
| 65 | Ser | Arg | Trp | Asp | Val | Asn | Phe | Ile | Gln | Ser | Leu | Leu | Ser | Asp | Tyr |
| Lys | Glu | Asp | Lys | His | Val | Ile | Arg | Ala | Ser | 75 | Glu | Leu | Val | Thr | 80 |
| | | | | 85 | | | | | 90 | | | | | | 95 |
| Lys | Met | Glu | Leu | Glu | Lys | Glu | Thr | Asp | Gln | Ile | Arg | Gln | Leu | Glu | Leu |
| | | | 100 | | | | | 105 | | | | | 110 | | |
| Ile | Asp | Asp | Leu | Gln | Arg | Met | Gly | Leu | Ser | Asp | His | Phe | Gln | Asn | Glu |
| | | | 115 | | | | 120 | | | | | 125 | | | |
| Phe | Lys | Glu | Ile | Leu | Ser | Ser | Ile | Tyr | Leu | Asp | His | His | Tyr | Tyr | Lys |
| | 130 | | | | | 135 | | | | | 140 | | | | |
| Asn | Pro | Phe | Pro | Lys | Glu | Glu | Arg | Asp | Leu | Tyr | Ser | Thr | Ser | Leu | Ala |
| 145 | | | | | 150 | | | | | 155 | | | | | 160 |
| Phe | Arg | Leu | Leu | Arg | Glu | His | Gly | Phe | Gln | Val | Ala | Gln | Glu | Val | Phe |
| | | | | 165 | | | | | 170 | | | | | 175 | |
| Asp | Ser | Phe | Lys | Asn | Glu | Glu | Gly | Glu | Phe | Lys | Glu | Ser | Leu | Ser | Asp |
| | | | 180 | | | | | 185 | | | | | 190 | | |
| Asp | Thr | Arg | Gly | Leu | Leu | Gln | Leu | Tyr | Glu | Ala | Ser | Phe | Leu | Leu | Thr |
| | | 195 | | | | | 200 | | | | | 205 | | | |
| Glu | Gly | Glu | Thr | Thr | Leu | Glu | Ser | Ala | Arg | Glu | Phe | Ala | Thr | Lys | Phe |
| | 210 | | | | | 215 | | | | | 220 | | | | |
| Leu | Glu | Glu | Lys | Val | Asn | Glu | Gly | Gly | Val | Asp | Gly | Asp | Leu | Leu | Thr |
| 225 | | | | | 230 | | | | | 235 | | | | | 240 |
| Arg | Ile | Ala | Tyr | Ser | Leu | Asp | Ile | Pro | Leu | His | Trp | Arg | Ile | Lys | Arg |
| | | | | 245 | | | | | 250 | | | | | 255 | |
| Pro | Asn | Ala | Pro | Val | Trp | Ile | Glu | Trp | Tyr | Arg | Lys | Arg | Pro | Asp | Met |
| | | | 260 | | | | | 265 | | | | | 270 | | |
| Asn | Pro | Val | Val | Leu | Glu | Leu | Ala | Ile | Leu | Asp | Leu | Asn | Ile | Val | Gln |
| | | 275 | | | | | 280 | | | | | 285 | | | |
| Ala | Gln | Phe | Gln | Glu | Glu | Leu | Lys | Glu | Ser | Phe | Arg | Trp | Trp | Arg | Asn |
| | 290 | | | | | 295 | | | | | 300 | | | | |
| Thr | Gly | Phe | Val | Glu | Lys | Leu | Pro | Phe | Ala | Arg | Asp | Arg | Leu | Val | Glu |
| 305 | | | | | 310 | | | | | 315 | | | | | 320 |
| Cys | Tyr | Phe | Trp | Asn | Thr | Gly | Ile | Ile | Glu | Pro | Arg | Gln | His | Ala | Ser |
| | | | | 325 | | | | | 330 | | | | | 335 | |
| Ala | Arg | Ile | Met | Met | Gly | Lys | Val | Asn | Ala | Leu | Ile | Thr | Val | Ile | Asp |
| | | | 340 | | | | | 345 | | | | | 350 | | |
| Asp | Ile | Tyr | Asp | Val | Tyr | Gly | Thr | Leu | Glu | Glu | Leu | Glu | Gln | Phe | Thr |
| | | 355 | | | | | 360 | | | | | 365 | | | |
| Asp | Leu | Ile | Arg | Arg | Trp | Asp | Ile | Asn | Ser | Ile | Asp | Gln | Leu | Pro | Asp |
| | 370 | | | | | 375 | | | | | 380 | | | | |
| Tyr | Met | Gln | Leu | Cys | Phe | Leu | Ala | Leu | Asn | Asn | Phe | Val | Asp | Asp | Thr |
| 385 | | | | | 390 | | | | | 395 | | | | | 400 |
| Ser | Tyr | Asp | | | | | | | | | | | | | |

Arg Val Thr Asp Ser Phe Thr Lys Glu Thr Val Asp Ser Leu Tyr Lys
 465 470 475 480
 Tyr His Asp Leu Val Arg Trp Ser Ser Phe Val Leu Arg Leu Ala Asp
 485 490 495
 Asp Leu Gly Thr Ser Val Glu Glu Val Ser Arg Gly Asp Val Pro Lys
 500 505 510
 Ser Leu Gln Cys Tyr Met Ser Asp Tyr Asn Ala Ser Glu Ala Glu Ala
 515 520 525
 Arg Lys His Val Lys Trp Leu Ile Ala Glu Val Trp Lys Lys Met Asn
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 Ala Glu Arg Val Ser Lys Asp Ser Pro Phe Gly Lys Asp Phe Ile Gly
 545 550 555 560
 Cys Ala Val Asp Leu Gly Arg Met Ala Gln Leu Met Tyr His Asn Gly
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 Thr Leu Phe Glu Pro Phe Ala
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<210> 23
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 <212> DNA
 <213> *Salvia officinalis*

<220>
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 <223> 1,8-cineole synthase

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 Met Ser Ser Leu Ile Met Gln Val Val Ile Pro Lys Pro
 1 5 10

 gcc aaa att ttt cac aat aac tta ttc agc gtg att tca aaa cga cat 99
 Ala Lys Ile Phe His Asn Asn Leu Phe Ser Val Ile Ser Lys Arg His
 15 20 25

 cgt ttc agt act aca atc acc act cgt ggt ggc agg tgg gca cat tgc 147
 Arg Phe Ser Thr Thr Ile Thr Thr Arg Gly Gly Arg Trp Ala His Cys
 30 35 40 45

 tca cta caa atg ggt aat gag atc caa act gga cga cga act gga ggc 195
 Ser Leu Gln Met Gly Asn Glu Ile Gln Thr Gly Arg Arg Thr Gly Gly
 50 55 60

 tac cag cct acc ctt tgg gat ttc agc acc att caa ttg ttc gac tct 243
 Tyr Gln Pro Thr Leu Trp Asp Phe Ser Thr Ile Gln Leu Phe Asp Ser
 65 70 75

 gag tat aag gaa gag aag cac ttg atg agg gcc gca ggt atg ata gcc 291
 Glu Tyr Lys Glu Glu Lys His Leu Met Arg Ala Ala Gly Met Ile Ala
 80 85 90

| | |
|---|-----|
| caa gtg aat atg ttg ttg cag gaa gaa gta gat tcg att caa cgg ttg | 339 |
| Gln Val Asn Met Leu Leu Gln Glu Glu Val Asp Ser Ile Gln Arg Leu | |
| 95 100 105 | |
| gag ttg att gat gac cta cga agg ctg ggt ata tct tgc cat ttt gac | 387 |
| Glu Leu Ile Asp Asp Leu Arg Arg Leu Gly Ile Ser Cys His Phe Asp | |
| 110 115 120 125 | |
| cgc gag atc gtt gaa ata tta aac tca aaa tat tat acc aac aat gag | 435 |
| Arg Glu Ile Val Glu Ile Leu Asn Ser Lys Tyr Tyr Thr Asn Asn Glu | |
| 130 135 140 | |
| ata gat gaa agt gat cta tac tca aca gcc ctt aga ttc aag ctc cta | 483 |
| Ile Asp Glu Ser Asp Leu Tyr Ser Thr Ala Leu Arg Phe Lys Leu Leu | |
| 145 150 155 | |
| aga caa tac gat ttt agc gtc tct caa gag gta ttt gat tgt ttc aag | 531 |
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| Asn Asp Lys Gly Thr Asp Phe Lys Pro Ser Leu Val Asp Asp Thr Arg | |
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| Gly Leu Leu Gln Leu Tyr Glu Ala Ser Phe Leu Ser Ala Gln Gly Glu | |
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| gaa acc cta cat ctt gcc aga gat ttt gct act aaa ttt ctg cat aaa | 675 |
| Glu Thr Leu His Leu Ala Arg Asp Phe Ala Thr Lys Phe Leu His Lys | |
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| Arg Val Leu Val Asp Lys Asp Ile Asn Leu Leu Ser Ser Ile Glu Arg | |
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| Ala Leu Glu Leu Pro Thr His Trp Arg Val Gln Met Pro Asn Ala Arg | |
| 240 245 250 | |
| tcc ttc att gat gct tat aag agg aga ccc gac atg aat ccg act gtg | 819 |
| Ser Phe Ile Asp Ala Tyr Lys Arg Arg Pro Asp Met Asn Pro Thr Val | |
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| cta gaa cta gct aaa ttg gac ttc aat atg gtt caa gca caa ttt caa | 867 |
| Leu Glu Leu Ala Lys Leu Asp Phe Asn Met Val Gln Ala Gln Phe Gln | |
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| Gln Glu Leu Lys Glu Ala Ser Arg Trp Trp Asn Ser Thr Gly Leu Val | |
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| Thr Thr Gly Val Val Glu Arg Arg Glu His Gly Tyr Glu Arg Ile Met | |
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| ctc acc aaa ata aat gct ctt gtt aca aca ata gac gat gtc ttt gat | 1059 |
| Leu Thr Lys Ile Asn Ala Leu Val Thr Thr Ile Asp Asp Val Phe Asp | |
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| Ile Tyr Gly Thr Leu Glu Glu Leu Gln Leu Phe Thr Thr Ala Ile Gln | |
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| Arg Trp Asp Ile Glu Ser Met Lys Gln Leu Pro Pro Tyr Met Gln Ile | |
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| Cys Tyr Leu Ala Leu Phe Asn Phe Val Asn Glu Met Ala Tyr Asp Thr | |
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| ctt agg gat aaa ggt ttc aac tcc acc cca tat cta cga aaa gcg tgg | 1251 |
| Leu Arg Asp Lys Gly Phe Asn Ser Thr Pro Tyr Leu Arg Lys Ala Trp | |
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| Val Asp Leu Val Glu Ser Tyr Leu Ile Glu Ala Lys Trp Tyr Tyr Met | |
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| Gly His Lys Pro Ser Leu Glu Glu Tyr Met Lys Asn Ser Trp Ile Ser | |
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| atc gga ggc atc ccc att cta tct cat cta ttt ttc cgg cta aca gat | 1395 |
| Ile Gly Gly Ile Pro Ile Leu Ser His Leu Phe Phe Arg Leu Thr Asp | |
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| Ser Ile Glu Glu Glu Asp Ala Glu Ser Met His Lys Tyr His Asp Ile | |
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| Val Arg Ala Ser Cys Thr Ile Leu Arg Leu Ala Asp Asp Met Gly Thr | |
| 480 485 490 | |
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| tac atg aat gag aag aat gct tcg gaa gaa gaa gcg cga gag cat gtg | 1587 |

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 Met Gly Asn Glu Ile Gln Thr Gly Arg Arg Thr Gly Gly Tyr Gln Pro
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 Thr Leu Trp Asp Phe Ser Thr Ile Gln Leu Phe Asp Ser Glu Tyr Lys
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 Glu Glu Lys His Leu Met Arg Ala Ala Gly Met Ile Ala Gln Val Asn
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 Asp Asp Leu Arg Arg Leu Gly Ile Ser Cys His Phe Asp Arg Glu Ile
 115 120 125
 Val Glu Ile Leu Asn Ser Lys Tyr Tyr Thr Asn Asn Glu Ile Asp Glu
 130 135 140
 Ser Asp Leu Tyr Ser Thr Ala Leu Arg Phe Lys Leu Leu Arg Gln Tyr
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| Asp | Phe | Ser | Val | Ser | Gln | Glu | Val | Phe | Asp | Cys | Phe | Lys | Asn | Asp | Lys |
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| Gly | Thr | Asp | Phe | Lys | Pro | Ser | Leu | Val | Asp | Asp | Thr | Arg | Gly | Leu | Leu |
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| Gln | Leu | Tyr | Glu | Ala | Ser | Phe | Leu | Ser | Ala | Gln | Gly | Glu | Glu | Thr | Leu |
| | | 195 | | | | | 200 | | | | | 205 | | | |
| His | Leu | Ala | Arg | Asp | Phe | Ala | Thr | Lys | Phe | Leu | His | Lys | Arg | Val | Leu |
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| Val | Asp | Lys | Asp | Ile | Asn | Leu | Leu | Ser | Ser | Ile | Glu | Arg | Ala | Leu | Glu |
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| Leu | Pro | Thr | His | Trp | Arg | Val | Gln | Met | Pro | Asn | Ala | Arg | Ser | Phe | Ile |
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| Asp | Ala | Tyr | Lys | Arg | Arg | Pro | Asp | Met | Asn | Pro | Thr | Val | Leu | Glu | Leu |
| | | | 260 | | | | | 265 | | | | | 270 | | |
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| Lys | Gly | Phe | Asn | Ser | Thr | Pro | Tyr | Leu | Arg | Lys | Ala | Trp | Val | Asp | Leu |
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| Glu | Val | Glu | Arg | Gly | Asp | Val | Pro | Lys | Ser | Val | Gln | Cys | Tyr | Met | Asn |
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43

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| Lys | Gly | Glu | Asp | Thr | Leu | Glu | Leu | Ala | Arg | Glu | Phe | Ala | Thr | Lys | Cys | |
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| ctg | cag | aaa | aaa | ctt | gat | gaa | ggg | ggg | aat | gaa | att | gat | gag | aat | cta | 721 |
| Leu | Gln | Lys | Lys | Leu | Asp | Glu | Gly | Gly | Asn | Glu | Ile | Asp | Glu | Asn | Leu | |
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| Gln | Ser | Val | Glu | Ala | Arg | Trp | Phe | Ile | Asp | Ala | Tyr | Ala | Arg | Arg | Pro | |
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| Asp | Met | Asn | Pro | Leu | Ile | Phe | Glu | Leu | Ala | Lys | Leu | Asn | Phe | Asn | Ile | |
| 270 | | | | | 275 | | | | 280 | | | | | | 285 | |
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| Ser | Arg | Leu | Cys | Phe | Pro | Glu | Lys | Leu | Pro | Phe | Val | Arg | Asp | Arg | Leu | |
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| Val | Glu | Ser | Phe | Phe | Trp | Ala | Val | Gly | Met | Phe | Glu | Pro | His | Gln | His | |
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| Gly | Tyr | Gln | Arg | Lys | Met | Ala | Ala | Thr | Ile | Ile | Val | Leu | Ala | Thr | Val | |
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| ata | gat | gat | att | tac | gat | gtg | tat | ggg | aca | cta | gat | gaa | cta | gaa | cta | 1105 |
| Ile | Asp | Asp | Ile | Tyr | Asp | Val | Tyr | Gly | Thr | Leu | Asp | Glu | Leu | Glu | Leu | |
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| | | | | | | | | | | | | | | | | |
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| Tyr | Leu | Arg | Lys | Ser | Val | Val | Asp | Leu | Val | Glu | Ala | Tyr | Phe | His | Glu | |
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| Ala | Lys | Trp | Tyr | His | Ser | Gly | Tyr | Thr | Pro | Ser | Leu | Asp | Glu | Tyr | Leu | |
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| Asn | Ile | Ala | Lys | Ile | Ser | Val | Ala | Ser | Pro | Ala | Ile | Ile | Ser | Pro | Thr | |
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| Leu | Tyr | Gln | Tyr | His | Asp | Ile | Leu | Cys | Leu | Ala | Gly | Ile | Ile | Leu | Arg | |
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| Leu | Pro | Asp | Asp | Leu | Gly | Thr | Ser | Tyr | Phe | Glu | Leu | Ala | Arg | Gly | Asp | |
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| gtg | ccg | aaa | aca | atc | cag | tgc | tac | atg | aag | gaa | aca | aat | gct | agt | gag | 1585 |
| Val | Pro | Lys | Thr | Ile | Gln | Cys | Tyr | Met | Lys | Glu | Thr | Asn | Ala | Ser | Glu | |
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| Glu | Glu | Ala | Val | Glu | His | Val | Lys | Phe | Leu | Ile | Arg | Glu | Ala | Trp | Lys | |
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| Asp | Met | Asn | Thr | Ala | Ile | Ala | Ala | Gly | Tyr | Pro | Phe | Pro | Asp | Gly | Met | |
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| Val | Ala | Gly | Ala | Ala | Asn | Ile | Gly | Arg | Val | Ala | Gln | Phe | Ile | Tyr | Leu | |
| | | 560 | | | | | 565 | | | | | 570 | | | | |
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| His | Gly | Asp | Gly | Phe | Gly | Val | Gln | His | Ser | Lys | Thr | Tyr | Glu | His | Ile | |

575 580 585

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Met Gln Leu Cys Tyr Trp Gly Val His Asn Tyr Ile Ser Asp Ala Ala
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Tyr Asp Ile Leu Lys Glu His Gly Phe Phe Cys Leu Gln Tyr Leu Arg
      405      410      415
Lys Ser Val Val Asp Leu Val Glu Ala Tyr Phe His Glu Ala Lys Trp
      420      425      430
Tyr His Ser Gly Tyr Thr Pro Ser Leu Asp Glu Tyr Leu Asn Ile Ala
      435      440      445
Lys Ile Ser Val Ala Ser Pro Ala Ile Ile Ser Pro Thr Tyr Phe Thr
      450      455      460
Phe Ala Asn Ala Ser His Asp Thr Ala Val Ile Asp Ser Leu Tyr Gln
 465      470      475      480
Tyr His Asp Ile Leu Cys Leu Ala Gly Ile Ile Leu Arg Leu Pro Asp
      485      490      495
Asp Leu Gly Thr Ser Tyr Phe Glu Leu Ala Arg Gly Asp Val Pro Lys
      500      505      510
Thr Ile Gln Cys Tyr Met Lys Glu Thr Asn Ala Ser Glu Glu Ala
      515      520      525
Val Glu His Val Lys Phe Leu Ile Arg Glu Ala Trp Lys Asp Met Asn
      530      535      540
Thr Ala Ile Ala Ala Gly Tyr Pro Phe Pro Asp Gly Met Val Ala Gly
 545      550      555      560
Ala Ala Asn Ile Gly Arg Val Ala Gln Phe Ile Tyr Leu His Gly Asp
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Gly Phe Gly Val Gln His Ser Lys Thr Tyr Glu His Ile Ala Gly Leu
      580      585      590
Leu Phe Glu Pro Tyr Ala
      595

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<210> 27

<211> 1959

<212> DNA

<213> Mentha x piperita

<220>

<221> CDS

<222> (71)...(1723)

<223> (E)-B-farnesene synthase

<400> 27

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| Met Ala Thr Asn Gly Val Val Ile Ser Cys Leu Arg Glu | |
| 1 5 10 | |
| gta agg cca cct atg acg aag cat gcg cca agc atg tgg act gat acc | 157 |
| Val Arg Pro Pro Met Thr Lys His Ala Pro Ser Met Trp Thr Asp Thr | |
| 15 20 25 | |
| ttt tct aac ttt tct ctt gac gat aag gaa caa caa aag tgc tca gaa | 205 |
| Phe Ser Asn Phe Ser Leu Asp Asp Lys Glu Gln Gln Lys Cys Ser Glu | |
| 30 35 40 45 | |
| acc atc gaa gca ctt aag caa gaa gca aga ggc atg ctt atg gct gca | 253 |
| Thr Ile Glu Ala Leu Lys Gln Glu Ala Arg Gly Met Leu Met Ala Ala | |
| 50 55 60 | |
| acc act cct ctc caa caa atg aca cta atc gac act ctc gag cgt ttg | 301 |
| Thr Thr Pro Leu Gln Gln Met Thr Leu Ile Asp Thr Leu Glu Arg Leu | |
| 65 70 75 | |
| gga ttg tct ttc cat ttt gag acg gag atc gaa tac aaa atc gaa cta | 349 |
| Gly Leu Ser Phe His Phe Glu Thr Glu Ile Glu Tyr Lys Ile Glu Leu | |
| 80 85 90 | |
| atc aac gct gca gaa gac gac ggc ttt gat ttg ttc gct act gct ctt | 397 |
| Ile Asn Ala Ala Glu Asp Asp Gly Phe Asp Leu Phe Ala Thr Ala Leu | |
| 95 100 105 | |
| cgt ttc cgt ttg ctc aga caa cat caa cgc cac gtt tct tgt gat gtt | 445 |
| Arg Phe Arg Leu Leu Arg Gln His Gln Arg His Val Ser Cys Asp Val | |
| 110 115 120 125 | |
| ttc gac aag ttc atc gac aaa gat ggc aag ttc gaa gaa tcc ctt agc | 493 |
| Phe Asp Lys Phe Ile Asp Lys Asp Gly Lys Phe Glu Glu Ser Leu Ser | |
| 130 135 140 | |
| aat aat gtt gaa ggc cta tta agc ttg tat gaa gca gct cat gtt ggg | 541 |
| Asn Asn Val Glu Gly Leu Leu Ser Leu Tyr Glu Ala Ala His Val Gly | |
| 145 150 155 | |
| ttt cgc gaa gaa aga ata tta caa gag gct gta aat ttt acg agg cat | 589 |
| Phe Arg Glu Glu Arg Ile Leu Gln Glu Ala Val Asn Phe Thr Arg His | |
| 160 165 170 | |
| cac ttg gaa gga gca gag tta gat cag tct cca tta ttg att aga gag | 637 |
| His Leu Glu Gly Ala Glu Leu Asp Gln Ser Pro Leu Leu Ile Arg Glu | |
| 175 180 185 | |
| aaa gtg aag cga gct ttg gag cac cct ctt cat agg gat ttc ccc att | 685 |
| Lys Val Lys Arg Ala Leu Glu His Pro Leu His Arg Asp Phe Pro Ile | |
| 190 195 200 205 | |
| gtc tat gca cgc ctt ttc atc tcc att tac gaa aag gat gac tct aga | 733 |

| | | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|------------|-----|-----|-----|-----|------------|-----|-----|-----|-----|------------|-----|-----|------|
| Val | Tyr | Ala | Arg | Leu 210 | Phe | Ile | Ser | Ile | Tyr 215 | Glu | Lys | Asp | Asp | Ser 220 | Arg | | |
| gat | gaa | tta | ctt | ctc | aag | cta | tcc | aaa | gtc | aac | ttc | aaa | ttc | atg | cag | | 781 |
| Asp | Glu | Leu | Leu | Leu | Lys | Leu | Ser | Lys | Val | Asn | Phe | Lys | Phe | Met | Gln | | |
| | | | 225 | | | | | 230 | | | | | 235 | | | | |
| aat | ttg | tat | aag | gaa | gag | ctc | tcc | caa | ctc | tcc | agg | tgg | tgg | aac | aca | | 829 |
| Asn | Leu | Tyr | Lys | Glu | Glu | Leu | Ser | Gln | Leu | Ser | Arg | Trp | Trp | Asn | Thr | | |
| | | 240 | | | | | 245 | | | | | 250 | | | | | |
| tgg | aat | ctg | aaa | tca | aaa | tta | cca | tat | gca | aga | gat | cga | gtc | gtg | gag | | 877 |
| Trp | Asn | Leu | Lys | Ser | Lys | Leu | Pro | Tyr | Ala | Arg | Asp | Arg | Val | Val | Glu | | |
| | 255 | | | | | 260 | | | | | 265 | | | | | | |
| gct | tat | gtt | tgg | gga | gta | ggt | tac | cat | tac | gaa | ccc | caa | tac | tca | tat | | 925 |
| Ala | Tyr | Val | Trp | Gly | Val | Gly | Tyr | His | Tyr | Glu | Pro | Gln | Tyr | Ser | Tyr | | |
| | 270 | | | | 275 | | | | | 280 | | | | | 285 | | |
| gtt | cga | atg | gga | ctt | gcc | aaa | ggc | gta | cta | att | tgt | gga | atc | atg | gac | | 973 |
| Val | Arg | Met | Gly | Leu | Ala | Lys | Gly | Val | Leu | Ile | Cys | Gly | Ile | Met | Asp | | |
| | | | | 290 | | | | | 295 | | | | | 300 | | | |
| gat | aca | tat | gat | aat | tat | gct | aca | ctc | aat | gaa | gct | caa | ctt | ttt | act | | 1021 |
| Asp | Thr | Tyr | Asp | Asn | Tyr | Ala | Thr | Leu | Asn | Glu | Ala | Gln | Leu | Phe | Thr | | |
| | | | 305 | | | | | 310 | | | | | 315 | | | | |
| caa | gtc | tta | gac | aag | tgg | gat | aga | gat | gaa | gct | gaa | cga | ctc | cca | gaa | | 1069 |
| Gln | Val | Leu | Asp | Lys | Trp | Asp | Arg | Asp | Glu | Ala | Glu | Arg | Leu | Pro | Glu | | |
| | | 320 | | | | | 325 | | | | | 330 | | | | | |
| tac | atg | aaa | atc | gtt | tat | cga | ttt | att | ttg | agt | ata | tat | gaa | aat | tat | | 1117 |
| Tyr | Met | Lys | Ile | Val | Tyr | Arg | Phe | Ile | Leu | Ser | Ile | Tyr | Glu | Asn | Tyr | | |
| | 335 | | | | | 340 | | | | | 345 | | | | | | |
| gaa | cgt | gat | gca | gcg | aaa | ctt | gga | aaa | agc | ttt | gca | gct | cct | tat | ttt | | 1165 |
| Glu | Arg | Asp | Ala | Ala | Lys | Leu | Gly | Lys | Ser | Phe | Ala | Ala | Pro | Tyr | Phe | | |
| | 350 | | | | 355 | | | | | 360 | | | | | 365 | | |
| aag | gaa | acc | gtg | aaa | caa | ctg | gca | agg | gca | ttt | aat | gag | gag | cag | aag | | 1213 |
| Lys | Glu | Thr | Val | Lys | Gln | Leu | Ala | Arg | Ala | Phe | Asn | Glu | Glu | Gln | Lys | | |
| | | | | 370 | | | | 375 | | | | | | 380 | | | |
| tgg | gtt | atg | gaa | agg | cag | cta | ccg | tca | ttc | caa | gac | tac | gta | aag | aat | | 1261 |
| Trp | Val | Met | Glu | Arg | Gln | Leu | Pro | Ser | Phe | Gln | Asp | Tyr | Val | Lys | Asn | | |
| | | | 385 | | | | | 390 | | | | | 395 | | | | |
| tca | gag | aaa | acc | agc | tgc | att | tat | acc | atg | ttt | gct | tct | atc | atc | cca | | 1309 |
| Ser | Glu | Lys | Thr | Ser | Cys | Ile | Tyr | Thr | Met | Phe | Ala | | Ser | Ile | Ile | Pro | |
| | | 400 | | | | | 405 | | | | | 410 | | | | | |
| ggc | ttg | aaa | tct | gtt | acc | caa | gaa | acc | att | gat | tgg | atc | aag | agt | gaa | | 1357 |
| Gly | Leu | Lys | Ser | Val | Thr | Gln | Glu | Thr | Ile | Asp | Trp | Ile | Lys | Ser | Glu | | |

| 415 | 420 | 425 | |
|---|-----|-----|------|
| ccc acc ctc gca aca tcg acc gct atg atc ggt cgg tat tgg aat gac | | | 1405 |
| Pro Thr Leu Ala Thr Ser Thr Ala Met Ile Gly Arg Tyr Trp Asn Asp | | | |
| 430 | 435 | 440 | 445 |
| acc agc tct cag ctc cgt gaa agc aaa gga ggg gaa atg ctg act gcg | | | 1453 |
| Thr Ser Ser Gln Leu Arg Glu Ser Lys Gly Gly Glu Met Leu Thr Ala | | | |
| | 450 | 455 | 460 |
| ttg gat ttc cac atg aaa gaa tat ggt ctg acg aag gaa gag gcg gca | | | 1501 |
| Leu Asp Phe His Met Lys Glu Tyr Gly Leu Thr Lys Glu Glu Ala Ala | | | |
| | 465 | 470 | 475 |
| tct aag ttt gaa gga ttg gtt gag gaa aca tgg aag gat ata aac aag | | | 1549 |
| Ser Lys Phe Glu Gly Leu Val Glu Glu Thr Trp Lys Asp Ile Asn Lys | | | |
| | 480 | 485 | 490 |
| gaa ttc ata gcc aca act aat tat aat gtg ggt aga gaa att gcc atc | | | 1597 |
| Glu Phe Ile Ala Thr Thr Asn Tyr Asn Val Gly Arg Glu Ile Ala Ile | | | |
| | 495 | 500 | 505 |
| aca ttc ctc aac tac gct cgg ata tgt gaa gcc agt tac agc aaa act | | | 1645 |
| Thr Phe Leu Asn Tyr Ala Arg Ile Cys Glu Ala Ser Tyr Ser Lys Thr | | | |
| | 510 | 515 | 520 |
| gac gga gac gct tat tca gat cct aat gtt gcc aag gca aat gtc gtt | | | 1693 |
| Asp Gly Asp Ala Tyr Ser Asp Pro Asn Val Ala Lys Ala Asn Val Val | | | |
| | 530 | 535 | 540 |
| gct ctc ttt gtt gat gcc ata gtc ttt tga tttgcataat caaagaccct | | | 1743 |
| Ala Leu Phe Val Asp Ala Ile Val Phe * | | | |
| | 545 | 550 | |
| ataattataa ttatatgtgt ttaagaaact aataagcttg ctttatgtat agttgtcaat | | | 1803 |
| tgaataataa tgtattaatt agtagagtta agaagttata aagaataaag aggagctggt | | | 1863 |
| agacgtaaac aagaaataat gtgtcaaaat aacttcaact ttttcaagaa taaagaattg | | | 1923 |
| gaagagacca atatatacaa aaaaaaaaaa aaaaaa | | | 1959 |

<210> 28

<211> 550

<212> PRT

<213> Mentha x piperita

<400> 28

| | |
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| Pro Met Thr Lys His Ala Pro Ser Met Trp Thr Asp Thr Phe Ser Asn | 10 |
| | 15 |
| Phe Ser Leu Asp Asp Lys Glu Gln Gln Lys Cys Ser Glu Thr Ile Glu | 20 |
| | 25 |
| Ala Leu Lys Gln Glu Ala Arg Gly Met Leu Met Ala Ala Thr Thr Pro | 30 |
| | 35 |
| | 40 |
| | 45 |
| | 50 |
| | 55 |
| | 60 |

| | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| Leu | Gln | Gln | Met | Thr | Leu | Ile | Asp | Thr | Leu | Glu | Arg | Leu | Gly | Leu | Ser |
| 65 | | | | | 70 | | | | | 75 | | | | | 80 |
| Phe | His | Phe | Glu | Thr | Glu | Ile | Glu | Tyr | Lys | Ile | Glu | Leu | Ile | Asn | Ala |
| | | | | 85 | | | | | 90 | | | | | | 95 |
| Ala | Glu | Asp | Asp | Gly | Phe | Asp | Leu | Phe | Ala | Thr | Ala | Leu | Arg | Phe | Arg |
| | | | 100 | | | | | 105 | | | | | 110 | | |
| Leu | Leu | Arg | Gln | His | Gln | Arg | His | Val | Ser | Cys | Asp | Val | Phe | Asp | Lys |
| | | 115 | | | | | 120 | | | | | 125 | | | |
| Phe | Ile | Asp | Lys | Asp | Gly | Lys | Phe | Glu | Glu | Ser | Leu | Ser | Asn | Asn | Val |
| | 130 | | | | | 135 | | | | | 140 | | | | |
| Glu | Gly | Leu | Leu | Ser | Leu | Tyr | Glu | Ala | Ala | His | Val | Gly | Phe | Arg | Glu |
| 145 | | | | | 150 | | | | | 155 | | | | | 160 |
| Glu | Arg | Ile | Leu | Gln | Glu | Ala | Val | Asn | Phe | Thr | Arg | His | His | Leu | Glu |
| | | | | 165 | | | | 170 | | | | | | | 175 |
| Gly | Ala | Glu | Leu | Asp | Gln | Ser | Pro | Leu | Ile | Arg | Glu | Lys | Val | Lys | |
| | | | 180 | | | | | 185 | | | | 190 | | | |
| Arg | Ala | Leu | Glu | His | Pro | Leu | His | Arg | Asp | Phe | Pro | Ile | Val | Tyr | Ala |
| | 195 | | | | | | 200 | | | | | 205 | | | |
| Arg | Leu | Phe | Ile | Ser | Ile | Tyr | Glu | Lys | Asp | Asp | Ser | Arg | Asp | Glu | Leu |
| | 210 | | | | | 215 | | | | | 220 | | | | |
| Leu | Leu | Lys | Leu | Ser | Lys | Val | Asn | Phe | Lys | Phe | Met | Gln | Asn | Leu | Tyr |
| 225 | | | | | 230 | | | | | 235 | | | | | 240 |
| Lys | Glu | Glu | Leu | Ser | Gln | Leu | Ser | Arg | Trp | Trp | Asn | Thr | Trp | Asn | Leu |
| | | | | 245 | | | | | 250 | | | | | 255 | |
| Lys | Ser | Lys | Leu | Pro | Tyr | Ala | Arg | Asp | Arg | Val | Val | Glu | Ala | Tyr | Val |
| | | | 260 | | | | | 265 | | | | | 270 | | |
| Trp | Gly | Val | Gly | Tyr | His | Tyr | Glu | Pro | Gln | Tyr | Ser | Tyr | Val | Arg | Met |
| | 275 | | | | | | 280 | | | | | 285 | | | |
| Gly | Leu | Ala | Lys | Gly | Val | Leu | Ile | Cys | Gly | Ile | Met | Asp | Asp | Thr | Tyr |
| | 290 | | | | | 295 | | | | | 300 | | | | |
| Asp | Asn | Tyr | Ala | Thr | Leu | Asn | Glu | Ala | Gln | Leu | Phe | Thr | Gln | Val | Leu |
| 305 | | | | | 310 | | | | | 315 | | | | | 320 |
| Asp | Lys | Trp | Asp | Arg | Asp | Glu | Ala | Glu | Arg | Leu | Pro | Glu | Tyr | Met | Lys |
| | | | | 325 | | | | 330 | | | | | | 335 | |
| Ile | Val | Tyr | Arg | Phe | Ile | Leu | Ser | Ile | Tyr | Glu | Asn | Tyr | Glu | Arg | Asp |
| | | | 340 | | | | | 345 | | | | | 350 | | |
| Ala | Ala | Lys | Leu | Gly | Lys | Ser | Phe | Ala | Ala | Pro | Tyr | Phe | Lys | Glu | Thr |
| | | 355 | | | | | 360 | | | | | 365 | | | |
| Val | Lys | Gln | Leu | Ala | Arg | Ala | Phe | Asn | Glu | Glu | Gln | Lys | Trp | Val | Met |
| | 370 | | | | | 375 | | | | | 380 | | | | |
| Glu | Arg | Gln | Leu | Pro | Ser | Phe | Gln | Asp | Tyr | Val | Lys | Asn | Ser | Glu | Lys |
| 385 | | | | | 390 | | | | | 395 | | | | | 400 |
| Thr | Ser | Cys | Ile | Tyr | Thr | Met | Phe | Ala | Ser | Ile | Ile | Pro | Gly | Leu | Lys |
| | | | 405 | | | | | 410 | | | | | 415 | | |
| Ser | Val | Thr | Gln | Glu | Thr | Ile | Asp | Trp | Ile | Lys | Ser | Glu | Pro | Thr | Leu |
| | | | 420 | | | | | 425 | | | | | 430 | | |
| Ala | Thr | Ser | Thr | Ala | Met | Ile | Gly | Arg | Tyr | Trp | Asn | Asp | Thr | Ser | Ser |
| | | 435 | | | | | 440 | | | | | 445 | | | |
| Gln | Leu | Arg | Glu | Ser | Lys | Gly | Gly | Glu | Met | Leu | Thr | Ala | Leu | Asp | Phe |
| | 450 | | | | | 455 | | | | | 460 | | | | |
| His | Met | Lys | Glu | Tyr | Gly | Leu | Thr | Lys | Glu | Glu | Ala | Ala | Ser | Lys | Phe |
| 465 | | | | | 470 | | | | | 475 | | | | | 480 |
| Glu | Gly | Leu | Val | Glu | Glu | Thr | Trp | Lys | Asp | Ile | Asn | Lys | Glu | Phe | Ile |

Ala Thr Thr Asn Tyr Asn Val Gly Arg Glu Ile Ala Ile Thr Phe Leu
 500 505 510
 Asn Tyr Ala Arg Ile Cys Glu Ala Ser Tyr Ser Lys Thr Asp Gly Asp
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 Ala Tyr Ser Asp Pro Asn Val Ala Lys Ala Asn Val Val Ala Leu Phe
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<211> 2196

<212> DNA

<213> *Abies grandis*

<220>

<221> CDS

<222> (69)...(1952)

<223> myrcene synthase

<400> 29

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| tgccg | gcacg | agg | tat | ctt | gag | ctt | cct | cat | atag | gcc | aac | acat | atc | atat | caa | agg | 60 |
| gag | caaga | atg | gct | ctg | ggt | tct | atc | tca | cgc | ttg | gct | tcg | aaa | tct | tgc | | 110 |
| | Met | Ala | Leu | Val | Ser | Ile | Ser | Pro | Leu | Ala | Ser | Lys | Ser | Cys | | | |
| | 1 | | | | 5 | | | | | | 10 | | | | | | |
| | | | | | | | | | | | | | | | | | |
| ctg | cgc | aag | tcg | ttg | atc | agt | tca | att | cat | gaa | cat | aag | cct | ccc | tat | | 158 |
| Leu | Arg | Lys | Ser | Leu | Ile | Ser | Ser | Ile | His | Glu | His | Lys | Pro | Pro | Tyr | | |
| 15 | | | | | 20 | | | | | 25 | | | | | 30 | | |
| | | | | | | | | | | | | | | | | | |
| aga | aca | atc | cca | aat | ctt | gga | atg | cgt | agg | cga | ggg | aaa | tct | gtc | acg | | 206 |
| Arg | Thr | Ile | Pro | Asn | Leu | Gly | Met | Arg | Arg | Arg | Gly | Lys | Ser | Val | Thr | | |
| | | | | 35 | | | | | 40 | | | | | | 45 | | |
| | | | | | | | | | | | | | | | | | |
| cct | tcc | atg | agc | atc | agt | ttg | gcc | acc | gct | gca | cct | gat | gat | ggg | gta | | 254 |
| Pro | Ser | Met | Ser | Ile | Ser | Leu | Ala | Thr | Ala | Ala | Pro | Asp | Asp | Gly | Val | | |
| | | | 50 | | | | | 55 | | | | | 60 | | | | |
| | | | | | | | | | | | | | | | | | |
| caa | aga | cgc | ata | ggg | gac | tac | cat | tcc | aat | atc | tgg | gac | gat | gat | ttc | | 302 |
| Gln | Arg | Arg | Ile | Gly | Asp | Tyr | His | Ser | Asn | Ile | Trp | Asp | Asp | Asp | Phe | | |
| | | 65 | | | | | 70 | | | | | 75 | | | | | |
| | | | | | | | | | | | | | | | | | |
| ata | cag | tct | cta | tca | acg | cct | tat | ggg | gaa | ccc | tct | tac | cag | gaa | cgt | | 350 |
| Ile | Gln | Ser | Leu | Ser | Thr | Pro | Tyr | Gly | Glu | Pro | Ser | Tyr | Gln | Glu | Arg | | |
| | 80 | | | | | 85 | | | | | 90 | | | | | | |
| | | | | | | | | | | | | | | | | | |
| gct | gag | aga | tta | att | gtg | gag | gta | aag | aag | ata | ttc | aat | tca | atg | tac | | 398 |
| Ala | Glu | Arg | Leu | Ile | Val | Glu | Val | Lys | Lys | Ile | Phe | Asn | Ser | Met | Tyr | | |
| | 95 | | | | 100 | | | | | 105 | | | | | 110 | | |
| | | | | | | | | | | | | | | | | | |
| ctg | gat | gat | gga | aga | tta | atg | agt | tcc | ttt | aat | gat | ctc | atg | caa | cgc | | 446 |
| Leu | Asp | Asp | Gly | Arg | Leu | Met | Ser | Ser | Phe | Asn | Asp | Leu | Met | Gln | Arg | | |
| | | | | 115 | | | | | 120 | | | | | 125 | | | |

| | |
|---|------|
| ctt tgg ata gtc gat agc gtt gaa cgt ttg ggg ata gct aga cat ttc Leu Trp Ile Val Asp Ser Val Glu Arg Leu Gly Ile Ala Arg His Phe 130 135 140 | 494 |
| aag aac gag ata aca tca gct ctg gat tat gtt ttc cgt tac tgg gag Lys Asn Glu Ile Thr Ser Ala Leu Asp Tyr Val Phe Arg Tyr Trp Glu 145 150 155 | 542 |
| gaa aac ggc att gga tgt ggg aga gac agt att gtt act gat ctc aac Glu Asn Gly Ile Gly Cys Gly Arg Asp Ser Ile Val Thr Asp Leu Asn 160 165 170 | 590 |
| tca act gcg ttg ggg ttt cga act ctt cga tta cac ggg tac act gta Ser Thr Ala Leu Gly Phe Arg Thr Leu Arg Leu His Gly Tyr Thr Val 175 180 185 190 | 638 |
| tct cca gag gtt tta aaa gct ttt caa gat caa aat gga cag ttt gta Ser Pro Glu Val Leu Lys Ala Phe Gln Asp Gln Asn Gly Gln Phe Val 195 200 205 | 686 |
| tgc tcc ccc ggt cag aca gag ggt gag atc aga agc gtt ctt aac tta Cys Ser Pro Gly Gln Thr Glu Gly Glu Ile Arg Ser Val Leu Asn Leu 210 215 220 | 734 |
| tat cgg gct tcc ctc att gcc ttc cct ggt gag aaa gtt atg gaa gaa Tyr Arg Ala Ser Leu Ile Ala Phe Pro Gly Glu Lys Val Met Glu Glu 225 230 235 | 782 |
| gct gaa atc ttc tcc aca aga tat ttg aaa gaa gct cta caa aag att Ala Glu Ile Phe Ser Thr Arg Tyr Leu Lys Glu Ala Leu Gln Lys Ile 240 245 250 | 830 |
| cca gtc tcc gct ctt tca caa gag ata aag ttt gtt atg gaa tat ggc Pro Val Ser Ala Leu Ser Gln Glu Ile Lys Phe Val Met Glu Tyr Gly 255 260 265 270 | 878 |
| tgg cac aca aat ttg cca aga ttg gaa gca aga aat tac ata gac aca Trp His Thr Asn Leu Pro Arg Leu Glu Ala Arg Asn Tyr Ile Asp Thr 275 280 285 | 926 |
| ctt gag aaa gac acc agt gca tgg ctc aat aaa aat gct ggg aag aag Leu Glu Lys Asp Thr Ser Ala Trp Leu Asn Lys Asn Ala Gly Lys Lys 290 295 300 | 974 |
| ctt tta gaa ctt gca aaa ttg gag ttc aat ata ttt aac tcc tta caa Leu Leu Glu Leu Ala Lys Leu Glu Phe Asn Ile Phe Asn Ser Leu Gln 305 310 315 | 1022 |
| caa aag gaa tta caa tat ctt ttg aga tgg tgg aaa gag tcg gat ttg Gln Lys Glu Leu Gln Tyr Leu Leu Arg Trp Trp Lys Glu Ser Asp Leu 320 325 330 | 1070 |

| | |
|---|------|
| cct aaa ttg aca ttt gct cgg cat cgt cat gtg gaa ttc tac act ttg | 1118 |
| Pro Lys Leu Thr Phe Ala Arg His Arg His Val Glu Phe Tyr Thr Leu | |
| 335 340 345 350 | |
| gcc tct tgt att gcc att gac cca aaa cat tct gca ttc aga cta ggc | 1166 |
| Ala Ser Cys Ile Ala Ile Asp Pro Lys His Ser Ala Phe Arg Leu Gly | |
| 355 360 365 | |
| ttc gcc aaa atg tgt cat ctt gtc aca gtt ttg gac gat att tac gac | 1214 |
| Phe Ala Lys Met Cys His Leu Val Thr Val Leu Asp Asp Ile Tyr Asp | |
| 370 375 380 | |
| act ttt gga acg att gac gag ctt gaa ctc ttc aca tct gca att aag | 1262 |
| Thr Phe Gly Thr Ile Asp Glu Leu Glu Leu Phe Thr Ser Ala Ile Lys | |
| 385 390 395 | |
| aga tgg aat tca tca gag ata gaa cac ctt cca gaa tat atg aaa tgt | 1310 |
| Arg Trp Asn Ser Ser Glu Ile Glu His Leu Pro Glu Tyr Met Lys Cys | |
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| gtg tac atg gtc gtg ttt gaa act gta aat gaa ctg aca cga gag gcg | 1358 |
| Val Tyr Met Val Val Phe Glu Thr Val Asn Glu Leu Thr Arg Glu Ala | |
| 415 420 425 430 | |
| gag aag act caa ggg aga aac act ctc aac tat gtt cga aag gct tgg | 1406 |
| Glu Lys Thr Gln Gly Arg Asn Thr Leu Asn Tyr Val Arg Lys Ala Trp | |
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| gag gct tat ttt gat tca tat atg gaa gaa gca aaa tgg atc tct aat | 1454 |
| Glu Ala Tyr Phe Asp Ser Tyr Met Glu Glu Ala Lys Trp Ile Ser Asn | |
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| ggt tat ctg cca atg ttt gaa gag tac cat gag aat ggg aaa gtg agc | 1502 |
| Gly Tyr Leu Pro Met Phe Glu Glu Tyr His Glu Asn Gly Lys Val Ser | |
| 465 470 475 | |
| tct gca tat cgc gta gca aca ttg caa ccc atc ctc act ttg aat gca | 1550 |
| Ser Ala Tyr Arg Val Ala Thr Leu Gln Pro Ile Leu Thr Leu Asn Ala | |
| 480 485 490 | |
| tgg ctt cct gat tac atc ttg aag gga att gat ttt cca tcc agg ttc | 1598 |
| Trp Leu Pro Asp Tyr Ile Leu Lys Gly Ile Asp Phe Pro Ser Arg Phe | |
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| aat gat ttg gca tcg tcc ttc ctt cgg cta cga ggt gac aca cgc tgc | 1646 |
| Asn Asp Leu Ala Ser Ser Phe Leu Arg Leu Arg Gly Asp Thr Arg Cys | |
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| tac aag gcc gat agg gat cgt ggt gaa gaa gct tcg tgt ata tca tgt | 1694 |
| Tyr Lys Ala Asp Arg Asp Arg Gly Glu Glu Ala Ser Cys Ile Ser Cys | |
| 530 535 540 | |
| tat atg aaa gac aat cct gga tca acc gaa gaa gat gcc ctc aat cat | 1742 |

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| Tyr | Met | Lys | Asp | Asn | Pro | Gly | Ser | Thr | Glu | Glu | Asp | Ala | Leu | Asn | His | | |
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| atc | aat | gcc | atg | gtc | aat | gac | ata | atc | aaa | gaa | tta | aat | tgg | gaa | ctt | 1790 | |
| Ile | Asn | Ala | Met | Val | Asn | Asp | Ile | Ile | Lys | Glu | Leu | Asn | Trp | Glu | Leu | | |
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| cta | aga | tcc | aac | gac | aat | att | cca | atg | ctg | gcc | aag | aaa | cat | gct | ttt | 1838 | |
| Leu | Arg | Ser | Asn | Asp | Asn | Ile | Pro | Met | Leu | Ala | Lys | Lys | His | Ala | Phe | | |
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| Asp | Ile | Thr | Arg | Ala | Leu | His | His | Leu | Tyr | Ile | Tyr | Arg | Asp | Gly | Phe | | |
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| Ser | Val | Ala | Asn | Lys | Glu | Thr | Lys | Lys | Leu | Val | Met | Glu | Thr | Leu | Leu | | |
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| gaa | tct | atg | ctt | ttt | taa | ctataac | cat | atccata | ata | ataagct | cat | | | | | 1982 | |
| Glu | Ser | Met | Leu | Phe | * | | | | | | | | | | | | |
| | | | 625 | | | | | | | | | | | | | | |
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| Ile | Val | Asp | Ser | Val | Glu | Arg | Leu | Gly | Ile | Ala | Arg | His | Phe | Lys | Asn | | |
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| | | | | | | | | | | | | | | |
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| Gly | Ile | Gly | Cys | Gly | Arg | Asp | Ser | Ile | Val | Thr | Asp | Leu | Asn | Ser |
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| Glu | Val | Leu | Lys | Ala | Phe | Gln | Asp | Gln | Asn | Gly | Gln | Phe | Val | Cys |
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| Leu | Thr | Phe | Ala | Arg | His | Arg | His | Val | Glu | Phe | Tyr | Thr | Leu | Ala |
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| Gly | Thr | Ile | Asp | Glu | Leu | Glu | Leu | Phe | Thr | Ser | Ala | Ile | Lys | Arg |
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| Asn | Ser | Ser | Glu | Ile | Glu | His | Leu | Pro | Glu | Tyr | Met | Lys | Cys | Val |
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| Met | Val | Val | Phe | Glu | Thr | Val | Asn | Glu | Leu | Thr | Arg | Glu | Ala | Glu |
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| Thr | Gln | Gly | Arg | Asn | Thr | Leu | Asn | Tyr | Val | Arg | Lys | Ala | Trp | Glu |
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57

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| Ala | Phe | Ser | Thr | Ala | His | Leu | Glu | Ser | Ala | Ala | Pro | His | Leu | Lys | Ser | | |
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| Ser | Ile | Pro | Arg | Val | Glu | Thr | Arg | Tyr | Phe | Ile | Ser | Ile | Tyr | Glu | Glu | | |
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| Glu | Glu | Gln | Lys | Asn | Asp | Val | Leu | Leu | Gln | Phe | Ala | Lys | Leu | Asp | Phe | | |
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| Trp | Trp | Lys | Asp | Leu | Asp | Phe | Val | Thr | Thr | Leu | Pro | Tyr | Ala | Arg | Asp | | |
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| Tyr | Asn | Asp | Tyr | Glu | Met | Glu | Leu | Ser | Lys | Asp | Gly | Arg | Ser | Asp | Val | |
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| Val | His | Tyr | Ala | Lys | Glu | Arg | Met | Lys | Glu | Ile | Val | Arg | Asn | Tyr | Phe | |
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| gtg | gaa | gca | aaa | tgg | ttc | att | gaa | gga | tat | atg | ccg | cca | gtc | tct | gag | 1259 |
| Val | Glu | Ala | Lys | Trp | Phe | Ile | Glu | Gly | Tyr | Met | Pro | Pro | Val | Ser | Glu | |
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| Tyr | Leu | Ser | Asn | Ala | Leu | Ala | Thr | Ser | Thr | Tyr | Tyr | Leu | Leu | Thr | Thr | |
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| aca | tct | tat | ttg | ggc | atg | aag | tct | gct | aac | aag | caa | gat | ttt | gaa | tgg | 1355 |
| Thr | Ser | Tyr | Leu | Gly | Met | Lys | Ser | Ala | Asn | Lys | Gln | Asp | Phe | Glu | Trp | |
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| Leu | Ala | Lys | Asn | Pro | Lys | Ile | Leu | Glu | Ala | Asn | Val | Thr | Leu | Cys | Arg | |
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| gtc | ata | gat | gac | ata | gcc | acc | tat | gag | gtt | gag | aag | ggg | aga | ggg | cag | 1451 |
| Val | Ile | Asp | Asp | Ile | Ala | Thr | Tyr | Glu | Val | Glu | Lys | Gly | Arg | Gly | Gln | |
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| att | gcc | act | gga | att | gaa | tgt | tac | atg | aga | gat | tat | ggg | gta | tcc | aca | 1499 |
| Ile | Ala | Thr | Gly | Ile | Glu | Cys | Tyr | Met | Arg | Asp | Tyr | Gly | Val | Ser | Thr | |
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| gaa | aag | gcc | atg | gaa | aaa | ttc | caa | gaa | atg | gct | gag | aca | gca | tgg | aag | 1547 |
| Glu | Lys | Ala | Met | Glu | Lys | Phe | Gln | Glu | Met | Ala | Glu | Thr | Ala | Trp | Lys | |
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| Leu | Thr | Arg | Ile | Leu | Asn | Leu | Ala | Arg | Ile | Ile | Asp | Val | Thr | Tyr | Lys | |
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| cac | aat | caa | gat | gga | tac | act | cat | ccg | gaa | aaa | gta | cta | aaa | cct | cat | 1691 |
| His | Asn | Gln | Asp | Gly | Tyr | Thr | His | Pro | Glu | Lys | Val | Leu | Lys | Pro | His | |
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| 305 | Leu | Glu | Ile | Tyr | Thr | Asp | Ala | Ile | Gln | Arg | Trp | Asp | Ile | Ser | Gln | Ile |
| | Asp | Arg | Leu | Pro | Asp | Tyr | Met | Lys | Ile | Ser | Tyr | Lys | Ala | Leu | Leu | Asp |
| | Leu | Tyr | Asn | Asp | Tyr | Glu | Met | Glu | Leu | Ser | Lys | Asp | Gly | Arg | Ser | Asp |
| | Val | Val | His | Tyr | Ala | Lys | Glu | Arg | Met | Lys | Glu | Ile | Val | Arg | Asn | Tyr |
| | Phe | Val | Glu | Ala | Lys | Trp | Phe | Ile | Glu | Gly | Tyr | Met | Pro | Pro | Val | Ser |
| 385 | Glu | Tyr | Leu | Ser | Asn | Ala | Leu | Ala | Thr | Ser | Thr | Tyr | Tyr | Leu | Leu | Thr |
| | Thr | Thr | Ser | Tyr | Leu | Gly | Met | Lys | Ser | Ala | Asn | Lys | Gln | Asp | Phe | Glu |
| | Trp | Leu | Ala | Lys | Asn | Pro | Lys | Ile | Leu | Glu | Ala | Asn | Val | Thr | Leu | Cys |
| | Arg | Val | Ile | Asp | Asp | Ile | Ala | Thr | Tyr | Glu | Val | Glu | Lys | Gly | Arg | Gly |
| | Gln | Ile | Ala | Thr | Gly | Ile | Glu | Cys | Tyr | Met | Arg | Asp | Tyr | Gly | Val | Ser |
| 465 | Thr | Glu | Lys | Ala | Met | Glu | Lys | Phe | Gln | Glu | Met | Ala | Glu | Thr | Ala | Trp |
| | Lys | Asp | Val | Asn | Glu | Gly | Ile | Leu | Arg | Pro | Thr | Pro | Val | Ser | Thr | Glu |
| | Ile | Leu | Thr | Arg | Ile | Leu | Asn | Leu | Ala | Arg | Ile | Ile | Asp | Val | Thr | Tyr |
| | Lys | His | Asn | Gln | Asp | Gly | Tyr | Thr | His | Pro | Glu | Lys | Val | Leu | Lys | Pro |
| 530 | His | Ile | Ile | Ala | Leu | Leu | Val | Asp | Ser | Ile | Glu | Ile | | | | |
| 545 | | | | | | | | | | | | | | | | |

<210> 33
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<220>
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<222> (3596) ... (3889)

<400> 33

| | | | | | | | | | | | | |
|------------|-------------|-------------|-------------|-------------|-------------|------|-----|-----|-----|-----|-----|-----|
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| ttcgatttta | aggggaattgt | gccagcccct | agtttcgccc | ttgtttgtag | tgctttattt | 120 | | | | | | |
| taaaaaagta | aataataatag | aatatgtata | tatatatata | tataaaccaa | agtgaagat | 180 | | | | | | |
| gaaaatttat | ataaatgatc | gctgcaagct | tcaagctcac | aataatatga | ttctttacca | 240 | | | | | | |
| tcaagaaaca | ttgggtgcttt | atacagagaa | aagaaaaact | ttggctcctcc | tcgtagctaa | 300 | | | | | | |
| tattttaaca | atttaatttt | tatataataa | atttttaaca | attatttcac | attttttaaa | 360 | | | | | | |
| tatattcatg | ttgaatgtag | cagtatatag | ttatattagt | tatgctcata | aattttggat | 420 | | | | | | |
| gcattagatt | ttccttatgt | aatttgataa | caatgattat | tattttttact | tctaacaaat | 480 | | | | | | |
| aattaaatat | ttttttgttg | attcgataaa | tatcattatt | ttttaaatga | tttaaaatat | 540 | | | | | | |
| aaaaataata | atagattcga | ccgaacgctc | accctattga | gtgagtatat | caattattag | 600 | | | | | | |
| aatttaatta | aaaaaggaaa | ccaaatatag | ccggcttaat | tttgtttaat | attaatttat | 660 | | | | | | |
| gtgtggaaat | tcacttaaaa | acagagtcca | tggtgcttaa | catattatat | attaaaccat | 720 | | | | | | |
| ttcctattaa | taaattttatg | aacgagagtt | acatccttct | aaattcattt | tacttagagg | 780 | | | | | | |
| cggagtataa | tatttttatgt | agtagttatt | ctttttactat | ataaataaat | aaataaaatt | 840 | | | | | | |
| ttaatcgctt | gtgtattatg | attgattcag | ctgaatcaaa | gttggataaa | tatttttaatt | 900 | | | | | | |
| tgggatccca | atttaattgag | attgggtttga | ttttgggttg | taaatatttt | ttattaattt | 960 | | | | | | |
| tagataaatt | attggaagtt | ggagtcaaaa | ttgaccgtct | cagctaatta | tacaaataat | 1020 | | | | | | |
| aataatatag | agaaatgggt | atattgctca | acactcacat | ttactacgtc | agcaatagtc | 1080 | | | | | | |
| agacagactg | ctaagtaaac | aatgtacact | caattcgagt | caaacaaatc | ctttatccca | 1140 | | | | | | |
| agattctaaa | ataatgtgtt | tgaggcacca | attttgaagg | atagaaagtg | gaaacaaaca | 1200 | | | | | | |
| aaaggatatt | aaaaaacaag | gaaattttctc | actgtatttg | catatttttc | tccttccagt | 1260 | | | | | | |
| ataattaaaa | tacgtgcaat | ttacgttgta | ctttgttgac | tcctatctta | tacctataaa | 1320 | | | | | | |
| tacatgcaac | aattgcacac | atcgtctcat | ccaaaacctg | tgtttttaaac | actaaacagt | 1380 | | | | | | |
| aagcaaaggc | agcaaattaa | tctttgaatt | atttgcttcc | aaaaccctac | acttttctct | 1440 | | | | | | |
| caacacatcc | tagaaa atg | gct tca caa | gct tct caa | gtt ctt gct | tca ccc | 1492 | | | | | | |
| | Met | Ala | Ser | Gln | Ala | Ser | Gln | Val | Leu | Ala | Ser | Pro |
| | 1 | | | | 5 | | | | | 10 | | |

| | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|
| cat | ccc | gcō | att | tca | tcc | gaa | aat | cga | ccc | aag | gct | gat | ttt | cat | ccc | 1540 |
| His | Pro | Ala | Ile | Ser | Ser | Glu | Asn | Arg | Pro | Lys | Ala | Asp | Phe | His | Pro | |
| | 15 | | | | | 20 | | | | | 25 | | | | | |

| | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------------|------|--|--|
| ggt | att | tgg | ggt | gat | atg | ttc | atc | atc | tgt | cct | gat | acg | gtaatctata | 1589 | | |
| Gly | Ile | Trp | Gly | Asp | Met | Phe | Ile | Ile | Cys | Pro | Asp | Thr | | | | |
| | 30 | | | | 35 | | | | 40 | | | | | | | |

| | | | | | | | | | | | | | | | | |
|------------|------------|------------|------------|------------|------------|---------|-----|------|-----|-----|-----|-----|--|--|--|--|
| atttttttct | tactttctct | tttatcgatt | tttaagtttt | ttggagattt | catggaaaag | 1649 | | | | | | | | | | |
| cattatacgt | acttgagcag | gat atc | gat gct | gca act | gaa tta | caa tat | gaa | 1702 | | | | | | | | |
| | | Asp | Ile | Asp | Ala | Ala | Thr | Glu | Leu | Gln | Tyr | Glu | | | | |
| | | | 45 | | | | | 50 | | | | | | | | |

| | |
|---|------|
| gaa tta aaa gca caa gtg agg aag atg att atg gaa cct gtt gat gat | 1750 |
| Glu Leu Lys Ala Gln Val Arg Lys Met Ile Met Glu Pro Val Asp Asp | |
| 55 60 65 | |
| tca aac caa aag ttg ccc ttc att gat gct gtt caa aga tta ggt gtg | 1798 |
| Ser Asn Gln Lys Leu Pro Phe Ile Asp Ala Val Gln Arg Leu Gly Val | |
| 70 75 80 | |
| agt tat cat ttt gag aaa gag att gaa gat gaa cta gag aat att tac | 1846 |
| Ser Tyr His Phe Glu Lys Glu Ile Glu Asp Glu Leu Glu Asn Ile Tyr | |
| 85 90 95 100 | |
| cgt gac acc aac aac aat gat gcg gac acc gat ctc tac act aca gct | 1894 |
| Arg Asp Thr Asn Asn Asn Asp Ala Asp Thr Asp Leu Tyr Thr Thr Ala | |
| 105 110 115 | |
| ctt cga ttc cgg tta ctt aga gag cat ggc ttc gat att tct tgt | 1939 |
| Leu Arg Phe Arg Leu Leu Arg Glu His Gly Phe Asp Ile Ser Cys | |
| 120 125 130 | |
| ggtaattaag tcttaaactt tcataactct tcttatccat ttatcaatta atattatcaa | 1999 |
| actttacatt aataatcatc tgtacaatac ttcaatatat atatatttat tgatgaaact | 2059 |
| aatgtttgat gatgattttg ggtgcttgac ca gat gca ttc aac aag ttc aaa | 2112 |
| Asp Ala Phe Asn Lys Phe Lys | |
| 135 | |
| gat gag gca ggg aac ttc aag gca tca ttg aca agt gat gtg caa ggg | 2160 |
| Asp Glu Ala Gly Asn Phe Lys Ala Ser Leu Thr Ser Asp Val Gln Gly | |
| 140 145 150 | |
| ttg ttg gaa ctt tat gaa gct tcc tat atg agg gtc cat ggg gaa gat | 2208 |
| Leu Leu Glu Leu Tyr Glu Ala Ser Tyr Met Arg Val His Gly Glu Asp | |
| 155 160 165 170 | |
| ata ctt gat gaa gcc att tct ttc acc act gct caa ctt aca ctt gct | 2256 |
| Ile Leu Asp Glu Ala Ile Ser Phe Thr Thr Ala Gln Leu Thr Leu Ala | |
| 175 180 185 | |
| cta cca act tta cac cat cct tta tcg gaa cag gtc ggc cat gcc tta | 2304 |
| Leu Pro Thr Leu His His Pro Leu Ser Glu Gln Val Gly His Ala Leu | |
| 190 195 200 | |
| aag cag tct atc cga agg ggc ttg cca agg gtt gag gcc cgg aat ttc | 2352 |
| Lys Gln Ser Ile Arg Arg Gly Leu Pro Arg Val Glu Ala Arg Asn Phe | |
| 205 210 215 | |
| att tcg ata tac caa gat tta gaa tcc cat aac aaa tcg ttg ctt caa | 2400 |
| Ile Ser Ile Tyr Gln Asp Leu Glu Ser His Asn Lys Ser Leu Leu Gln | |
| 220 225 230 | |
| ttt gca aag att gat ttc aac ttg ttg cag ctt ttg cat agg aaa gag | 2448 |
| Phe Ala Lys Ile Asp Phe Asn Leu Leu Gln Leu Leu His Arg Lys Glu | |

| | | | | |
|--|-----|-----------------------------|-------------|------|
| 235 | 240 | 245 | 250 | |
| cta agt gag atc tgc agg taagtgtttg gagatcttta aagctatgaa | | | | 2496 |
| Leu Ser Glu Ile Cys Arg | | | | |
| | 255 | | | |
| gtctaataact atttcaattg atcacacgac tggtgctgac attttatgat gcttttttta | | | | 2556 |
| gg tgg tgg aaa gat tta gac ttt aca aga aaa cta cca ttt gca aga | | | | 2603 |
| Trp Trp Lys Asp Leu Asp Phe Thr Arg Lys Leu Pro Phe Ala Arg | | | | |
| | 260 | 265 | 270 | |
| gat aga gtg gtt gaa ggc tat ttt tgg ata atg gga gtt tac ttt gaa | | | | 2651 |
| Asp Arg Val Val Glu Gly Tyr Phe Trp Ile Met Gly Val Tyr Phe Glu | | | | |
| | 275 | 280 | 285 | |
| ccc caa tac tct ctt ggt aga aag atg ttg aca aaa gtc ata gca atg | | | | 2699 |
| Pro Gln Tyr Ser Leu Gly Arg Lys Met Leu Thr Lys Val Ile Ala Met | | | | |
| | 290 | 295 | 300 | |
| gct tcc att gtt gat gat act tat gat tca tat gca acc tat gat gaa | | | | 2747 |
| Ala Ser Ile Val Asp Asp Thr Tyr Asp Ser Tyr Ala Thr Tyr Asp Glu | | | | |
| | 305 | 310 | 315 | |
| ctc att ccc tat aca aat gca att gaa ggtgagattt tttttccttt | | | | 2794 |
| Leu Ile Pro Tyr Thr Asn Ala Ile Glu | | | | |
| | 320 | 325 | | |
| cctccaaaaa aaaaaaaagt ttttgagatc cccaagaat aggggaaaaat atatgttttt | | | | 2854 |
| aaacgtttagg atattcactc caacttgcag ttgctcatat tttaatggtg atagtatgaa | | | | 2914 |
| ctaaccaggc taagttttag attcaaatta accctgaaat tgtgtttt agg tgg gat | | | | 2971 |
| | | | Arg Trp Asp | |
| | | | 330 | |
| att aaa tgc atg aac caa ctc ccg aat tac atg aaa ata agc tac aag | | | | 3019 |
| Ile Lys Cys Met Asn Gln Leu Pro Asn Tyr Met Lys Ile Ser Tyr Lys | | | | |
| | 335 | 340 | 345 | |
| gca cta tta gat gtt tat gaa gaa atg gaa cag ctg ttg gca aat caa | | | | 3067 |
| Ala Leu Leu Asp Val Tyr Glu Glu Met Glu Gln Leu Leu Ala Asn Gln | | | | |
| | 350 | 355 | 360 | |
| ggg aga cag tac cga gtt gag tat gcg aaa aag gcg gtatgtaatg | | | | 3113 |
| Gly Arg Gln Tyr Arg Val Glu Tyr Ala Lys Lys Ala | | | | |
| | 365 | 370 | 375 | |
| atacaatagt atgatatgct ttaatcataa acgtataaaa tttgaaaatt acattagcaa | | | | 3173 |
| tttgcttact tttttatgcc tttaatcctc ag atg ata cgt ctt gtt caa gct | | | | 3226 |
| | | Met Ile Arg Leu Val Gln Ala | | |
| | | | 380 | |
| tac ctt ttg gag gcc aaa tgg act cat caa aat tat aaa cca acc ttt | | | | 3274 |
| Tyr Leu Leu Glu Ala Lys Trp Thr His Gln Asn Tyr Lys Pro Thr Phe | | | | |
| | 385 | 390 | 395 | |

gag gaa ttt aga gat aat gca ttg cca acc tct ggc tat gcc atg ctt 3322
 Glu Glu Phe Arg Asp Asn Ala Leu Pro Thr Ser Gly Tyr Ala Met Leu
 400 405 410

gct ata acg gcg ttt gtc ggc atg ggc gaa gtt ata acc cct gag acc 3370
 Ala Ile Thr Ala Phe Val Gly Met Gly Glu Val Ile Thr Pro Glu Thr
 415 420 425 430

ttc aaa tgg gcc gcc agt gac ccc aag atc att aag gct tcc acc att 3418
 Phe Lys Trp Ala Ala Ser Asp Pro Lys Ile Ile Lys Ala Ser Thr Ile
 435 440 445

att tgc agg ttc atg gac gat att gct gaa cat aag gtatactata 3464
 Ile Cys Arg Phe Met Asp Asp Ile Ala Glu His Lys
 450 455

tattcatatt caagaattct aaaaatcgat tatgggtatat atatgcactt aaatctatat 3524
 catagaattg taaggcttct aggggttgca tttgctaagt taattaatat acatgggttca 3584
 tatgggtgca g ttc aac cat agg aga gaa gac gat tgc tca gcg atc gaa 3634
 Phe Asn His Arg Arg Glu Asp Asp Cys Ser Ala Ile Glu
 460 465 470

tgt tac atg aaa caa tat ggg gtg aca gcg cag gaa gca tac aat gaa 3682
 Cys Tyr Met Lys Gln Tyr Gly Val Thr Ala Gln Glu Ala Tyr Asn Glu
 475 480 485

ttc aac aaa cac att gag agt tca tgg aaa gat gta aat gaa gag ttc 3730
 Phe Asn Lys His Ile Glu Ser Ser Trp Lys Asp Val Asn Glu Glu Phe
 490 495 500

ttg aaa ccg aca gaa atg ccg aca ccc gtt ctt tgt cgt agc ctc aac 3778
 Leu Lys Pro Thr Glu Met Pro Thr Pro Val Leu Cys Arg Ser Leu Asn
 505 510 515

ctt gct agg gtt atg gat gta ctt tac aga gaa ggt gac ggt tat aca 3826
 Leu Ala Arg Val Met Asp Val Leu Tyr Arg Glu Gly Asp Gly Tyr Thr
 520 525 530 535

cat gtt ggg aaa gct gct aaa ggt ggg atc act tca tta ttg att gat 3874
 His Val Gly Lys Ala Ala Lys Gly Gly Ile Thr Ser Leu Leu Ile Asp
 540 545 550

cca ata caa att tga aattcaacat tggcttaaga ttactatga gataaaatta 3929
 Pro Ile Gln Ile *
 555

ataaggtttg tacaatgaag g 3950

<210> 34
 <211> 41
 <212> PRT
 <213> Gossypium arboreum

<400> 34
 Met Ala Ser Gln Ala Ser Gln Val Leu Ala Ser Pro His Pro Ala Ile
 1 5 10 15
 Ser Ser Glu Asn Arg Pro Lys Ala Asp Phe His Pro Gly Ile Trp Gly
 20 25 30
 Asp Met Phe Ile Ile Cys Pro Asp Thr
 35 40

<210> 35
 <211> 90
 <212> PRT
 <213> Gossypium arboreum

<400> 35
 Asp Ile Asp Ala Ala Thr Glu Leu Gln Tyr Glu Glu Leu Lys Ala Gln
 1 5 10 15
 Val Arg Lys Met Ile Met Glu Pro Val Asp Asp Ser Asn Gln Lys Leu
 20 25 30
 Pro Phe Ile Asp Ala Val Gln Arg Leu Gly Val Ser Tyr His Phe Glu
 35 40 45
 Lys Glu Ile Glu Asp Glu Leu Glu Asn Ile Tyr Arg Asp Thr Asn Asn
 50 55 60
 Asn Asp Ala Asp Thr Asp Leu Tyr Thr Thr Ala Leu Arg Phe Arg Leu
 65 70 75 80
 Leu Arg Glu His Gly Phe Asp Ile Ser Cys
 85 90

<210> 36
 <211> 125
 <212> PRT
 <213> Gossypium arboreum

<400> 36
 Asp Ala Phe Asn Lys Phe Lys Asp Glu Ala Gly Asn Phe Lys Ala Ser
 1 5 10 15
 Leu Thr Ser Asp Val Gln Gly Leu Leu Glu Leu Tyr Glu Ala Ser Tyr
 20 25 30
 Met Arg Val His Gly Glu Asp Ile Leu Asp Glu Ala Ile Ser Phe Thr
 35 40 45
 Thr Ala Gln Leu Thr Leu Ala Leu Pro Thr Leu His His Pro Leu Ser
 50 55 60
 Glu Gln Val Gly His Ala Leu Lys Gln Ser Ile Arg Arg Gly Leu Pro
 65 70 75 80
 Arg Val Glu Ala Arg Asn Phe Ile Ser Ile Tyr Gln Asp Leu Glu Ser
 85 90 95
 His Asn Lys Ser Leu Leu Gln Phe Ala Lys Ile Asp Phe Asn Leu Leu
 100 105 110
 Gln Leu Leu His Arg Lys Glu Leu Ser Glu Ile Cys Arg
 115 120 125

<210> 37
 <211> 72

<212> PRT

<213> Gossypium arboreum

<400> 37

| | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| Trp | Trp | Lys | Asp | Leu | Asp | Phe | Thr | Arg | Lys | Leu | Pro | Phe | Ala | Arg | Asp |
| 1 | | | | 5 | | | | | 10 | | | | | 15 | |
| Arg | Val | Val | Glu | Gly | Tyr | Phe | Trp | Ile | Met | Gly | Val | Tyr | Phe | Glu | Pro |
| | | | 20 | | | | | 25 | | | | | 30 | | |
| Gln | Tyr | Ser | Leu | Gly | Arg | Lys | Met | Leu | Thr | Lys | Val | Ile | Ala | Met | Ala |
| | | 35 | | | | | 40 | | | | | 45 | | | |
| Ser | Ile | Val | Asp | Asp | Thr | Tyr | Asp | Ser | Tyr | Ala | Thr | Tyr | Asp | Glu | Leu |
| | 50 | | | | | 55 | | | | | 60 | | | | |
| Ile | Pro | Tyr | Thr | Asn | Ala | Ile | Glu | | | | | | | | |
| 65 | | | | | 70 | | | | | | | | | | |

<210> 38

<211> 47

<212> PRT

<213> Gossypium arboreum

<400> 38

| | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| Arg | Trp | Asp | Ile | Lys | Cys | Met | Asn | Gln | Leu | Pro | Asn | Tyr | Met | Lys | Ile |
| 1 | | | | 5 | | | | | 10 | | | | | 15 | |
| Ser | Tyr | Lys | Ala | Leu | Leu | Asp | Val | Tyr | Glu | Glu | Met | Glu | Gln | Leu | Leu |
| | | | 20 | | | | | 25 | | | | | 30 | | |
| Ala | Asn | Gln | Gly | Arg | Gln | Tyr | Arg | Val | Glu | Tyr | Ala | Lys | Lys | Ala | |
| | | 35 | | | | | 40 | | | | | 45 | | | |

<210> 39

<211> 83

<212> PRT

<213> Gossypium arboreum

<400> 39

| | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| Met | Ile | Arg | Leu | Val | Gln | Ala | Tyr | Leu | Leu | Glu | Ala | Lys | Trp | Thr | His |
| 1 | | | | 5 | | | | | 10 | | | | | 15 | |
| Gln | Asn | Tyr | Lys | Pro | Thr | Phe | Glu | Glu | Phe | Arg | Asp | Asn | Ala | Leu | Pro |
| | | | 20 | | | | | 25 | | | | | 30 | | |
| Thr | Ser | Gly | Tyr | Ala | Met | Leu | Ala | Ile | Thr | Ala | Phe | Val | Gly | Met | Gly |
| | | 35 | | | | | 40 | | | | | 45 | | | |
| Glu | Val | Ile | Thr | Pro | Glu | Thr | Phe | Lys | Trp | Ala | Ala | Ser | Asp | Pro | Lys |
| | 50 | | | | | 55 | | | | | 60 | | | | |
| Ile | Ile | Lys | Ala | Ser | Thr | Ile | Ile | Cys | Arg | Phe | Met | Asp | Asp | Ile | Ala |
| 65 | | | | | 70 | | | | | 75 | | | | | 80 |
| Glu | His | Lys | | | | | | | | | | | | | |

<210> 40

<211> 97

<212> PRT

<213> Gossypium arboreum

<400> 40

Phe Asn His Arg Arg Glu Asp Asp Cys Ser Ala Ile Glu Cys Tyr Met
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 Lys Gln Tyr Gly Val Thr Ala Gln Glu Ala Tyr Asn Glu Phe Asn Lys
 20 25 30
 His Ile Glu Ser Ser Trp Lys Asp Val Asn Glu Glu Phe Leu Lys Pro
 35 40 45
 Thr Glu Met Pro Thr Pro Val Leu Cys Arg Ser Leu Asn Leu Ala Arg
 50 55 60
 Val Met Asp Val Leu Tyr Arg Glu Gly Asp Gly Tyr Thr His Val Gly
 65 70 75 80
 Lys Ala Ala Lys Gly Gly Ile Thr Ser Leu Ile Asp Pro Ile Gln
 85 90 95
 Ile

<210> 41
 <211> 1994
 <212> DNA
 <213> Ricinus communis

<220>
 <221> CDS
 <222> (67)...(1869)
 <223> casbene synthase

<400> 41
 actcagcagc cgcctctcct accccaatta gcacagaaga ttggtggtt cctctccttg 60
 tgaaac atg gca ttg cca tca gct gct atg caa tcc aac cct gaa aag 108
 Met Ala Leu Pro Ser Ala Ala Met Gln Ser Asn Pro Glu Lys
 1 5 10
 ctt aac tta ttt cac aga ttg tca agc tta ccc acc act agc ttg gaa 156
 Leu Asn Leu Phe His Arg Leu Ser Ser Leu Pro Thr Thr Ser Leu Glu 30
 15 20 25
 tat ggc aat aat cgc ttc cct ttc ttt tcc tca tct gcc aag tca cac 204
 Tyr Gly Asn Asn Arg Phe Pro Phe Phe Ser Ser Ser Ala Lys Ser His 45
 35 40 45
 ttt aaa aaa cca act caa gca tgt tta tcc tca aca acc cac caa gaa 252
 Phe Lys Lys Pro Thr Gln Ala Cys Leu Ser Ser Thr Thr His Gln Glu 60
 50 55 60
 gtt cgt cca tta gca tac ttt cct cct act gtc tgg ggc aat cgc ttt 300
 Val Arg Pro Leu Ala Tyr Phe Pro Pro Thr Val Trp Gly Asn Arg Phe 75
 65 70 75
 gct tcc ttg acc ttc aat cca tcg gaa ttt gaa tcg tat gat gaa cgg 348
 Ala Ser Leu Thr Phe Asn Pro Ser Glu Phe Glu Ser Tyr Asp Glu Arg 80
 85 90
 gta att gtg ctg aag aaa aaa gtt aag gac ata tta att tca tct aca 396
 Val Ile Val Leu Lys Lys Lys Val Lys Asp Ile Leu Ile Ser Ser Thr

| 95 | 100 | 105 | 110 | |
|--|-----|-----|-----|------|
| agt gat tca gtg gag acc gtt att tta atc gac tta tta tgt cgg ctt Ser Asp Ser Val Glu Thr Val Ile Leu Ile Asp Leu Leu Cys Arg Leu | 115 | 120 | 125 | 444 |
| ggc gta tca tat cac ttt gaa aat gat att gaa gag cta cta agt aaa Gly Val Ser Tyr His Phe Glu Asn Asp Ile Glu Glu Leu Leu Ser Lys | 130 | 135 | 140 | 492 |
| atc ttc aac tcc cag cct gac ctt gtc gat gaa aaa gaa tgt gat ctc Ile Phe Asn Ser Gln Pro Asp Leu Val Asp Glu Lys Glu Cys Asp Leu | 145 | 150 | 155 | 540 |
| tac act gcg gca att gta ttc cga gtt ttc aga cag cat ggt ttt aaa Tyr Thr Ala Ala Ile Val Phe Arg Val Phe Arg Gln His Gly Phe Lys | 160 | 165 | 170 | 588 |
| atg tct tcg gat gtg ttt agc aaa ttc aag gac agt gat ggt aag ttc Met Ser Ser Asp Val Phe Ser Lys Phe Lys Asp Ser Asp Gly Lys Phe | 175 | 180 | 185 | 636 |
| aag gaa tcc cta cgg ggt gat gct aag ggt atg ctc agc ctt ttt gaa Lys Glu Ser Leu Arg Gly Asp Ala Lys Gly Met Leu Ser Leu Phe Glu | 195 | 200 | 205 | 684 |
| gct tcc cat cta agt gtg cat gga gaa gac att ctt gaa gaa gcc ttt Ala Ser His Leu Ser Val His Gly Glu Asp Ile Leu Glu Glu Ala Phe | 210 | 215 | 220 | 732 |
| gct ttc acc aag gat tac tta cag tcc tct gca gtt gag tta ttc cct Ala Phe Thr Lys Asp Tyr Leu Gln Ser Ser Ala Val Glu Leu Phe Pro | 225 | 230 | 235 | 780 |
| aat ctc aaa agg cat ata acg aac gcc cta gag cag cct ttc cac agt Asn Leu Lys Arg His Ile Thr Asn Ala Leu Glu Gln Pro Phe His Ser | 240 | 245 | 250 | 828 |
| ggc gtg ccg agg cta gag gcc agg aaa ttc atc gat cta tac gaa gct Gly Val Pro Arg Leu Glu Ala Arg Lys Phe Ile Asp Leu Tyr Glu Ala | 255 | 260 | 265 | 876 |
| gat att gaa tgc cgg aat gaa act ctg ctc gag ttt gca aag ttg gat Asp Ile Glu Cys Arg Asn Glu Thr Leu Leu Glu Phe Ala Lys Leu Asp | 275 | 280 | 285 | 924 |
| tat aat aga gtt cag tta ttg cac caa caa gag ctg tgc cag ttc tca Tyr Asn Arg Val Gln Leu Leu His Gln Gln Glu Leu Cys Gln Phe Ser | 290 | 295 | 300 | 972 |
| aag tgg tgg aaa gac ctg aat ctt gct tcg gat att cct tat gca aga Lys Trp Trp Lys Asp Leu Asn Leu Ala Ser Asp Ile Pro Tyr Ala Arg | 305 | 310 | 315 | 1020 |

| | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|
| gac | aga | atg | gca | gag | att | ttc | ttt | tgg | gca | gtc | gcg | atg | tac | ttt | gag | 1068 |
| Asp | Arg | Met | Ala | Glu | Ile | Phe | Phe | Trp | Ala | Val | Ala | Met | Tyr | Phe | Glu | |
| 320 | | | | | | 325 | | | | | 330 | | | | | |
| cct | gac | tat | gca | cac | acc | cga | atg | att | att | gcg | aag | gtt | gta | ttg | ctt | 1116 |
| Pro | Asp | Tyr | Ala | His | Thr | Arg | Met | Ile | Ile | Ala | Lys | Val | Val | Leu | Leu | |
| 335 | | | | | 340 | | | | | 345 | | | | | 350 | |
| ata | tca | cta | ata | gat | gat | aca | att | gat | gcg | tat | gca | aca | atg | gag | gaa | 1164 |
| Ile | Ser | Leu | Ile | Asp | Asp | Thr | Ile | Asp | Ala | Tyr | Ala | Thr | Met | Glu | Glu | |
| | | | | 355 | | | | | 360 | | | | | 365 | | |
| act | cat | att | ctt | gct | gaa | gca | gtc | gca | agg | tgg | gac | atg | agc | tgc | ctc | 1212 |
| Thr | His | Ile | Leu | Ala | Glu | Ala | Val | Ala | Arg | Trp | Asp | Met | Ser | Cys | Leu | |
| | | | 370 | | | | | 375 | | | | | 380 | | | |
| gag | aag | ctg | cca | gat | tac | atg | aaa | gtt | att | tat | aaa | cta | ttg | cta | aac | 1260 |
| Glu | Lys | Leu | Pro | Asp | Tyr | Met | Lys | Val | Ile | Tyr | Lys | Leu | Leu | Leu | Asn | |
| | | 385 | | | | | 390 | | | | | 395 | | | | |
| acc | ttc | tct | gaa | ttc | gag | aaa | gaa | ttg | acg | gcg | gaa | ggc | aag | tcc | tac | 1308 |
| Thr | Phe | Ser | Glu | Phe | Glu | Lys | Glu | Leu | Thr | Ala | Glu | Gly | Lys | Ser | Tyr | |
| | 400 | | | | | 405 | | | | | 410 | | | | | |
| agc | gtc | aaa | tac | gga | agg | gaa | gcg | ttt | caa | gaa | cta | gtg | aga | ggc | tac | 1356 |
| Ser | Val | Lys | Tyr | Gly | Arg | Glu | Ala | Phe | Gln | Glu | Leu | Val | Arg | Gly | Tyr | |
| 415 | | | | | 420 | | | | | 425 | | | | | 430 | |
| tac | ctg | gag | gct | gta | tgg | cgc | gac | gag | ggc | aaa | ata | cca | tcg | ttc | gat | 1404 |
| Tyr | Leu | Glu | Ala | Val | Trp | Arg | Asp | Glu | Gly | Lys | Ile | Pro | Ser | Phe | Asp | |
| | | | | 435 | | | | | 440 | | | | | 445 | | |
| gac | tac | ttg | tat | aat | gga | tcc | atg | acc | acc | gga | ttg | cct | ctc | gtc | tca | 1452 |
| Asp | Tyr | Leu | Tyr | Asn | Gly | Ser | Met | Thr | Thr | Gly | Leu | Pro | Leu | Val | Ser | |
| | | | 450 | | | | | 455 | | | | | 460 | | | |
| aca | gct | tct | ttc | atg | gga | gtt | caa | gaa | att | aca | ggc | ctc | aac | gaa | ttc | 1500 |
| Thr | Ala | Ser | Phe | Met | Gly | Val | Gln | Glu | Ile | Thr | Gly | Leu | Asn | Glu | Phe | |
| | | | 465 | | | | 470 | | | | | 475 | | | | |
| caa | tgg | ctg | gaa | act | aat | ccc | aaa | tta | agt | tat | gct | tcc | ggc | gca | ttc | 1548 |
| Gln | Trp | Leu | Glu | Thr | Asn | Pro | Lys | Leu | Ser | Tyr | Ala | Ser | Gly | Ala | Phe | |
| | 480 | | | | | 485 | | | | | 490 | | | | | |
| atc | cga | ctt | gtc | aac | gac | tta | act | tct | cat | gtg | act | gaa | caa | caa | aga | 1596 |
| Ile | Arg | Leu | Val | Asn | Asp | Leu | Thr | Ser | His | Val | Thr | Glu | Gln | Gln | Arg | |
| 495 | | | | | 500 | | | | | 505 | | | | | 510 | |
| gga | cac | gtt | gca | tct | tgc | atc | gac | tgc | tat | atg | aac | caa | cat | gga | gtt | 1644 |
| Gly | His | Val | Ala | Ser | Cys | Ile | Asp | Cys | Tyr | Met | Asn | Gln | His | Gly | Val | |
| | | | | 515 | | | | | 520 | | | | | 525 | | |

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tcc aaa gac gaa gca gtc aaa ata ctt caa aaa atg gct aca gat tgt      1692
Ser Lys Asp Glu Ala Val Lys Ile Leu Gln Lys Met Ala Thr Asp Cys
                    530                      535                      540

tgg aaa gaa att aat gaa gaa tgt atg agg cag agt caa gtg tca gtg      1740
Trp Lys Glu Ile Asn Glu Glu Cys Met Arg Gln Ser Gln Val Ser Val
                    545                      550                      555

ggg cac cta atg aga ata gtt aat ctg gca cgt ctt acg gat gtg agt      1788
Gly His Leu Met Arg Ile Val Asn Leu Ala Arg Leu Thr Asp Val Ser
                    560                      565                      570

tac aag tat gga gac ggt tac act gat tcc cag caa ttg aaa caa ttt      1836
Tyr Lys Tyr Gly Asp Gly Tyr Thr Asp Ser Gln Gln Leu Lys Gln Phe
575                      580                      585                      590

gtt aag gga ttg ttc gtt gat cca att tct att tgaactcaat aattcctttt      1889
Val Lys Gly Leu Phe Val Asp Pro Ile Ser Ile
                    595                      600

ttcattttgt acttcaataa gttataaatg acccgtgcac tagcgggtggt gattattgta      1949
tttaaattgc cttttaaatt aatatatgaa tcaagaattt tatag      1994

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<212> PRT
<213> Ricinus communis

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Leu Phe His Arg Leu Ser Ser Leu Pro Thr Thr Ser Leu Glu Tyr Gly
20      25      30
Asn Asn Arg Phe Pro Phe Phe Ser Ser Ser Ala Lys Ser His Phe Lys
35      40      45
Lys Pro Thr Gln Ala Cys Leu Ser Ser Thr Thr His Gln Glu Val Arg
50      55      60
Pro Leu Ala Tyr Phe Pro Pro Thr Val Trp Gly Asn Arg Phe Ala Ser
65      70      75      80
Leu Thr Phe Asn Pro Ser Glu Phe Glu Ser Tyr Asp Glu Arg Val Ile
85      90      95
Val Leu Lys Lys Lys Val Lys Asp Ile Leu Ile Ser Ser Thr Ser Asp
100     105     110
Ser Val Glu Thr Val Ile Leu Ile Asp Leu Leu Cys Arg Leu Gly Val
115     120     125
Ser Tyr His Phe Glu Asn Asp Ile Glu Glu Leu Leu Ser Lys Ile Phe
130     135     140
Asn Ser Gln Pro Asp Leu Val Asp Glu Lys Glu Cys Asp Leu Tyr Thr
145     150     155     160
Ala Ala Ile Val Phe Arg Val Phe Arg Gln His Gly Phe Lys Met Ser
165     170     175     180
Ser Asp Val Phe Ser Lys Phe Lys Asp Ser Asp Gly Lys Phe Lys Glu
180     185     190

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| | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| Ser | Leu | Arg | Gly | Asp | Ala | Lys | Gly | Met | Leu | Ser | Leu | Phe | Glu | Ala | Ser |
| | | 195 | | | | | 200 | | | | | 205 | | | |
| His | Leu | Ser | Val | His | Gly | Glu | Asp | Ile | Leu | Glu | Glu | Ala | Phe | Ala | Phe |
| | 210 | | | | | 215 | | | | | 220 | | | | |
| Thr | Lys | Asp | Tyr | Leu | Gln | Ser | Ser | Ala | Val | Glu | Leu | Phe | Pro | Asn | Leu |
| | 225 | | | | 230 | | | | | 235 | | | | | 240 |
| Lys | Arg | His | Ile | Thr | Asn | Ala | Leu | Glu | Gln | Pro | Phe | His | Ser | Gly | Val |
| | | | 245 | | | | | 250 | | | | | | 255 | |
| Pro | Arg | Leu | Glu | Ala | Arg | Lys | Phe | Ile | Asp | Leu | Tyr | Glu | Ala | Asp | Ile |
| | | 260 | | | | | 265 | | | | | | 270 | | |
| Glu | Cys | Arg | Asn | Glu | Thr | Leu | Leu | Glu | Phe | Ala | Lys | Leu | Asp | Tyr | Asn |
| | 275 | | | | | | 280 | | | | | 285 | | | |
| Arg | Val | Gln | Leu | Leu | His | Gln | Gln | Glu | Leu | Cys | Gln | Phe | Ser | Lys | Trp |
| | 290 | | | | 295 | | | | | | 300 | | | | |
| Trp | Lys | Asp | Leu | Asn | Leu | Ala | Ser | Asp | Ile | Pro | Tyr | Ala | Arg | Asp | Arg |
| | 305 | | | | 310 | | | | | 315 | | | | | 320 |
| Met | Ala | Glu | Ile | Phe | Phe | Trp | Ala | Val | Ala | Met | Tyr | Phe | Glu | Pro | Asp |
| | | | 325 | | | | | 330 | | | | | | 335 | |
| Tyr | Ala | His | Thr | Arg | Met | Ile | Ile | Ala | Lys | Val | Val | Leu | Leu | Ile | Ser |
| | | | 340 | | | | 345 | | | | | | 350 | | |
| Leu | Ile | Asp | Asp | Thr | Ile | Asp | Ala | Tyr | Ala | Thr | Met | Glu | Glu | Thr | His |
| | 355 | | | | | | 360 | | | | | 365 | | | |
| Ile | Leu | Ala | Glu | Ala | Val | Ala | Arg | Trp | Asp | Met | Ser | Cys | Leu | Glu | Lys |
| | 370 | | | | 375 | | | | | | 380 | | | | |
| Leu | Pro | Asp | Tyr | Met | Lys | Val | Ile | Tyr | Lys | Leu | Leu | Leu | Asn | Thr | Phe |
| | 385 | | | | 390 | | | | 395 | | | | | | 400 |
| Ser | Glu | Phe | Glu | Lys | Glu | Leu | Thr | Ala | Glu | Gly | Lys | Ser | Tyr | Ser | Val |
| | | | | 405 | | | | 410 | | | | | | 415 | |
| Lys | Tyr | Gly | Arg | Glu | Ala | Phe | Gln | Glu | Leu | Val | Arg | Gly | Tyr | Tyr | Leu |
| | | | 420 | | | | | 425 | | | | | 430 | | |
| Glu | Ala | Val | Trp | Arg | Asp | Glu | Gly | Lys | Ile | Pro | Ser | Phe | Asp | Asp | Tyr |
| | 435 | | | | | | 440 | | | | | 445 | | | |
| Leu | Tyr | Asn | Gly | Ser | Met | Thr | Thr | Gly | Leu | Pro | Leu | Val | Ser | Thr | Ala |
| | 450 | | | | | 455 | | | | | 460 | | | | |
| Ser | Phe | Met | Gly | Val | Gln | Glu | Ile | Thr | Gly | Leu | Asn | Glu | Phe | Gln | Trp |
| | 465 | | | | 470 | | | | | 475 | | | | | 480 |
| Leu | Glu | Thr | Asn | Pro | Lys | Leu | Ser | Tyr | Ala | Ser | Gly | Ala | Phe | Ile | Arg |
| | | | | 485 | | | | | 490 | | | | | 495 | |
| Leu | Val | Asn | Asp | Leu | Thr | Ser | His | Val | Thr | Glu | Gln | Gln | Arg | Gly | His |
| | | 500 | | | | | | 505 | | | | | 510 | | |
| Val | Ala | Ser | Cys | Ile | Asp | Cys | Tyr | Met | Asn | Gln | His | Gly | Val | Ser | Lys |
| | 515 | | | | | | 520 | | | | | 525 | | | |
| Asp | Glu | Ala | Val | Lys | Ile | Leu | Gln | Lys | Met | Ala | Thr | Asp | Cys | Trp | Lys |
| | 530 | | | | | 535 | | | | | 540 | | | | |
| Glu | Ile | Asn | Glu | Glu | Cys | Met | Arg | Gln | Ser | Gln | Val | Ser | Val | Gly | His |
| | 545 | | | | 550 | | | | | 555 | | | | | 560 |
| Leu | Met | Arg | Ile | Val | Asn | Leu | Ala | Arg | Leu | Thr | Asp | Val | Ser | Tyr | Lys |
| | | | | 565 | | | | | 570 | | | | | 575 | |
| Tyr | Gly | Asp | Gly | Tyr | Thr | Asp | Ser | Gln | Gln | Leu | Lys | Gln | Phe | Val | Lys |
| | | | 580 | | | | | 585 | | | | | 590 | | |
| Gly | Leu | Phe | Val | Asp | Pro | Ile | Ser | Ile | | | | | | | |
| | | 595 | | | | | 600 | | | | | | | | |

| | | | | | | | |
|---|--|-----|--|-----|--|-----|------|
| 155 | | 160 | | 165 | | 170 | |
| aac cag ctc cag gat gga tcg tgg ggt atc gaa tcg cac ttt agt tta | | | | | | | 579 |
| Asn Gln Leu Gln Asp Gly Ser Trp Gly Ile Glu Ser His Phe Ser Leu | | | | | | | |
| | | 175 | | 180 | | 185 | |
| tgc gat cga ttg ctt aac acg acc aat tct gtt atc gcc ctc tcg gtt | | | | | | | 627 |
| Cys Asp Arg Leu Leu Asn Thr Thr Asn Ser Val Ile Ala Leu Ser Val | | | | | | | |
| | | 190 | | 195 | | 200 | |
| tgg aaa aca ggg cac agc caa gta caa caa ggt gct gag ttt att gca | | | | | | | 675 |
| Trp Lys Thr Gly His Ser Gln Val Gln Gln Gly Ala Glu Phe Ile Ala | | | | | | | |
| | | 205 | | 210 | | 215 | |
| gag aat cta aga tta ctc aat gag gaa gat gag ttg tcc ccg gat ttc | | | | | | | 723 |
| Glu Asn Leu Arg Leu Leu Asn Glu Glu Asp Glu Leu Ser Pro Asp Phe | | | | | | | |
| | | 220 | | 225 | | 230 | |
| caa ata atc ttt cct gct ctg ctg caa aag gca aaa gcg ttg ggg atc | | | | | | | 771 |
| Gln Ile Ile Phe Pro Ala Leu Leu Gln Lys Ala Lys Ala Leu Gly Ile | | | | | | | |
| | | 235 | | 240 | | 245 | 250 |
| aat ctt cct tac gat ctt cca ttt atc aaa tat ttg tcg aca aca cgg | | | | | | | 819 |
| Asn Leu Pro Tyr Asp Leu Pro Phe Ile Lys Tyr Leu Ser Thr Thr Arg | | | | | | | |
| | | 255 | | 260 | | 265 | |
| gaa gcc agg ctt aca gat gtt tct gcg gca gca gac aat att cca gcc | | | | | | | 867 |
| Glu Ala Arg Leu Thr Asp Val Ser Ala Ala Ala Asp Asn Ile Pro Ala | | | | | | | |
| | | 270 | | 275 | | 280 | |
| aac atg ttg aat gcg ttg gaa ggt ctc gag gaa gtt att gac tgg aac | | | | | | | 915 |
| Asn Met Leu Asn Ala Leu Glu Gly Leu Glu Glu Val Ile Asp Trp Asn | | | | | | | |
| | | 285 | | 290 | | 295 | |
| aag att atg agg ttt caa agt aaa gat gga tct ttc ctg agc tcc cct | | | | | | | 963 |
| Lys Ile Met Arg Phe Gln Ser Lys Asp Gly Ser Phe Leu Ser Ser Pro | | | | | | | |
| | | 300 | | 305 | | 310 | |
| gcc tcc act gcc tgt gta ctg atg aat aca ggg gac gaa aaa tgt ttc | | | | | | | 1011 |
| Ala Ser Thr Ala Cys Val Leu Met Asn Thr Gly Asp Glu Lys Cys Phe | | | | | | | |
| | | 315 | | 320 | | 325 | 330 |
| act ttt ctc aac aat ctg ctc gac aaa ttc ggc ggc tgc gtg ccc tgt | | | | | | | 1059 |
| Thr Phe Leu Asn Asn Leu Leu Asp Lys Phe Gly Gly Cys Val Pro Cys | | | | | | | |
| | | 335 | | 340 | | 345 | |
| atg tat tcc atc gat ctg ctg gaa cgc ctt tcg ctg gtt gat aac att | | | | | | | 1107 |
| Met Tyr Ser Ile Asp Leu Leu Glu Arg Leu Ser Leu Val Asp Asn Ile | | | | | | | |
| | | 350 | | 355 | | 360 | |
| gag cat ctc gga atc ggt cgc cat ttc aaa caa gaa atc aaa gga gct | | | | | | | 1155 |
| Glu His Leu Gly Ile Gly Arg His Phe Lys Gln Glu Ile Lys Gly Ala | | | | | | | |
| | | 365 | | 370 | | 375 | |

| | |
|---|------|
| ctt gat tat gtc tac aga cat tgg agt gaa agg ggc atc ggt tgg ggc Leu Asp Tyr Val Tyr Arg His Trp Ser Glu Arg Gly Ile Gly Trp Gly 380 385 390 | 1203 |
| aga gac agc ctt gtt cca gat ctc aac acc aca gcc ctc ggc ctg cga Arg Asp Ser Leu Val Pro Asp Leu Asn Thr Thr Ala Leu Gly Leu Arg 395 400 405 410 | 1251 |
| act ctt cgc atg cac gga tac aat gtt tct tca gac gtt ttg aat aat Thr Leu Arg Met His Gly Tyr Asn Val Ser Ser Asp Val Leu Asn Asn 415 420 425 | 1299 |
| ttc aaa gat gaa aac ggg cgg ttc ttc tcc tct gcg ggc caa acc cat Phe Lys Asp Glu Asn Gly Arg Phe Phe Ser Ser Ala Gly Gln Thr His 430 435 440 | 1347 |
| gtc gaa ttg aga agc gtg gtg aat ctt ttc aga gct tcc gac ctt gca Val Glu Leu Arg Ser Val Val Asn Leu Phe Arg Ala Ser Asp Leu Ala 445 450 455 | 1395 |
| ttt cct gac gaa aga gct atg gac gat gct aga aaa ttt gca gaa cca Phe Pro Asp Glu Arg Ala Met Asp Asp Ala Arg Lys Phe Ala Glu Pro 460 465 470 | 1443 |
| tat ctt aga gag gca ctt gca acg aaa atc tca acc aat aca aaa cta Tyr Leu Arg Glu Ala Leu Ala Thr Lys Ile Ser Thr Asn Thr Lys Leu 475 480 485 490 | 1491 |
| ttc aaa gag att gag tac gtg gtg gag tac cct tgg cac atg agt atc Phe Lys Glu Ile Glu Tyr Val Val Glu Tyr Pro Trp His Met Ser Ile 495 500 505 | 1539 |
| cca cgc tta gaa gcc aga agt tat att gat tca tat gac gac aat tat Pro Arg Leu Glu Ala Arg Ser Tyr Ile Asp Ser Tyr Asp Asp Asn Tyr 510 515 520 | 1587 |
| gta tgg cag agg aag act cta tat aga atg cca tct ttg agt aat tca Val Trp Gln Arg Lys Thr Leu Tyr Arg Met Pro Ser Leu Ser Asn Ser 525 530 535 | 1635 |
| aaa tgt tta gaa ttg gca aaa ttg gac ttc aat atc gta caa tct ttg Lys Cys Leu Glu Leu Ala Lys Leu Asp Phe Asn Ile Val Gln Ser Leu 540 545 550 | 1683 |
| cat caa gag gag ttg aag ctt cta aca aga tgg tgg aag gaa tcc ggc His Gln Glu Glu Leu Lys Leu Leu Thr Arg Trp Trp Lys Glu Ser Gly 555 560 565 570 | 1731 |
| atg gca gat ata aat ttc act cga cac cga gtg gcg gag gtt tat ttt Met Ala Asp Ile Asn Phe Thr Arg His Arg Val Ala Glu Val Tyr Phe 575 580 585 | 1779 |

| | |
|---|------|
| tca tca gct aca ttt gaa ccc gaa tat tct gcc act aga att gcc ttc | 1827 |
| Ser Ser Ala Thr Phe Glu Pro Glu Tyr Ser Ala Thr Arg Ile Ala Phe | |
| 590 595 600 | |
| aca aaa att ggt tgt tta caa gtc ctt ttt gat gat atg gct gac atc | 1875 |
| Thr Lys Ile Gly Cys Leu Gln Val Leu Phe Asp Asp Met Ala Asp Ile | |
| 605 610 615 | |
| ttt gca aca cta gat gaa ttg aaa agt ttc act gag gga gta aag aga | 1923 |
| Phe Ala Thr Leu Asp Glu Leu Lys Ser Phe Thr Glu Gly Val Lys Arg | |
| 620 625 630 | |
| tgg gat aca tct ttg cta cat gag att cca gag tgt atg caa act tgc | 1971 |
| Trp Asp Thr Ser Leu Leu His Glu Ile Pro Glu Cys Met Gln Thr Cys | |
| 635 640 645 650 | |
| ttt aaa gtt tgg ttc aaa tta atg gaa gaa gta aat aat gat gtg gtt | 2019 |
| Phe Lys Val Trp Phe Lys Leu Met Glu Glu Val Asn Asn Asp Val Val | |
| 655 660 665 | |
| aag gta caa gga cgt gac atg ctc gct cac ata aga aaa ccc tgg gag | 2067 |
| Lys Val Gln Gly Arg Asp Met Leu Ala His Ile Arg Lys Pro Trp Glu | |
| 670 675 680 | |
| ttg tac ttc aat tgt tat gta caa gaa agg gag tgg ctt gaa gcc ggg | 2115 |
| Leu Tyr Phe Asn Cys Tyr Val Gln Glu Arg Glu Trp Leu Glu Ala Gly | |
| 685 690 695 | |
| tat ata cca act ttt gaa gag tac tta aag act tat gct ata tca gta | 2163 |
| Tyr Ile Pro Thr Phe Glu Glu Tyr Leu Lys Thr Tyr Ala Ile Ser Val | |
| 700 705 710 | |
| ggc ctt gga ccg tgt acc cta caa cca ata cta cta atg ggt gag ctt | 2211 |
| Gly Leu Gly Pro Cys Thr Leu Gln Pro Ile Leu Leu Met Gly Glu Leu | |
| 715 720 725 730 | |
| gtg aaa gat gat gtt gtt gag aaa gtg cac tat ccc tca aat atg ttt | 2259 |
| Val Lys Asp Asp Val Val Glu Lys Val His Tyr Pro Ser Asn Met Phe | |
| 735 740 745 | |
| gag ctt gta tcc ttg agc tgg cga cta aca aac gac acc aaa aca tat | 2307 |
| Glu Leu Val Ser Leu Ser Trp Arg Leu Thr Asn Asp Thr Lys Thr Tyr | |
| 750 755 760 | |
| cag gct gaa aag gct cga gga caa caa gcc tca ggc ata gca tgc tat | 2355 |
| Gln Ala Glu Lys Ala Arg Gly Gln Gln Ala Ser Gly Ile Ala Cys Tyr | |
| 765 770 775 | |
| atg aag gat aat cca gga gca act gag gaa gat gcc att aag cac ata | 2403 |
| Met Lys Asp Asn Pro Gly Ala Thr Glu Glu Asp Ala Ile Lys His Ile | |
| 780 785 790 | |
| tgt cgt gtt gtt gat cgg gcc ttg aaa gaa gca agc ttt gaa tat ttc | 2451 |

Cys Arg Val Val Asp Arg Ala Leu Lys Glu Ala Ser Phe Glu Tyr Phe
 795 800 805 810
 aaa cca tcc aat gat atc cca atg ggt tgc aag tcc ttt att ttt aac 2499
 Lys Pro Ser Asn Asp Ile Pro Met Gly Cys Lys Ser Phe Ile Phe Asn
 815 820 825
 ctt aga ttg tgt gtc caa atc ttt tac aag ttt ata gat ggg tac gga 2547
 Leu Arg Leu Cys Val Gln Ile Phe Tyr Lys Phe Ile Asp Gly Tyr Gly
 830 835 840
 atc gcc aat gag gag att aag gac tat ata aga aaa gtt tat att gat 2595
 Ile Ala Asn Glu Glu Ile Lys Asp Tyr Ile Arg Lys Val Tyr Ile Asp
 845 850 855
 cca att caa gta tga tatatcatgt aaaacctctt tttcatgata aattgactta 2650
 Pro Ile Gln Val *
 860
 ttattgtatt ggcaaaaaaaaa aaaaaaaaaa aaaaaaaaaa aaaaaaaaaa 2700

<210> 44
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<400> 44
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 35 40 45
 Ser Arg Gly Ser Gly Gly Pro Gly Pro Val Val Met Met Ser Ser Ser
 50 55 60
 Thr Gly Thr Ser Lys Val Val Ser Glu Thr Ser Thr Ile Val Asp
 65 70 75 80
 Asp Ile Pro Arg Leu Ser Ala Asn Tyr His Gly Asp Leu Trp His His
 85 90 95
 Asn Val Ile Gln Thr Leu Glu Thr Pro Phe Arg Glu Ser Ser Thr Tyr
 100 105 110
 Gln Glu Arg Ala Asp Glu Leu Val Val Lys Ile Lys Asp Met Phe Asn
 115 120 125
 Ala Leu Gly Asp Gly Asp Ile Ser Pro Ser Ala Tyr Asp Thr Ala Trp
 130 135 140
 Val Ala Arg Leu Ala Thr Ile Ser Ser Asp Gly Ser Glu Lys Pro Arg
 145 150 155 160
 Phe Pro Gln Ala Leu Asn Trp Val Phe Asn Asn Gln Leu Gln Asp Gly
 165 170 175
 Ser Trp Gly Ile Glu Ser His Phe Ser Leu Cys Asp Arg Leu Leu Asn
 180 185 190
 Thr Thr Asn Ser Val Ile Ala Leu Ser Val Trp Lys Thr Gly His Ser
 195 200 205

Gln Val Gln Gln Gly Ala Glu Phe Ile Ala Glu Asn Leu Arg Leu Leu
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 Asn Glu Glu Asp Glu Leu Ser Pro Asp Phe Gln Ile Ile Phe Pro Ala
 225 230 235 240
 Leu Leu Gln Lys Ala Lys Ala Leu Gly Ile Asn Leu Pro Tyr Asp Leu
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 Pro Phe Ile Lys Tyr Leu Ser Thr Thr Arg Glu Ala Arg Leu Thr Asp
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 Val Ser Ala Ala Ala Asp Asn Ile Pro Ala Asn Met Leu Asn Ala Leu
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 Glu Gly Leu Glu Glu Val Ile Asp Trp Asn Lys Ile Met Arg Phe Gln
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 Ser Lys Asp Gly Ser Phe Leu Ser Ser Pro Ala Ser Thr Ala Cys Val
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 Leu Met Asn Thr Gly Asp Glu Lys Cys Phe Thr Phe Leu Asn Asn Leu
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 Leu Asp Lys Phe Gly Gly Cys Val Pro Cys Met Tyr Ser Ile Asp Leu
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 Leu Glu Arg Leu Ser Leu Val Asp Asn Ile Glu His Leu Gly Ile Gly
 355 360 365
 Arg His Phe Lys Gln Glu Ile Lys Gly Ala Leu Asp Tyr Val Tyr Arg
 370 375 380
 His Trp Ser Glu Arg Gly Ile Gly Trp Gly Arg Asp Ser Leu Val Pro
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 Asp Leu Asn Thr Thr Ala Leu Gly Leu Arg Thr Leu Arg Met His Gly
 405 410 415
 Tyr Asn Val Ser Ser Asp Val Leu Asn Asn Phe Lys Asp Glu Asn Gly
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 Arg Phe Phe Ser Ser Ala Gly Gln Thr His Val Glu Leu Arg Ser Val
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 Val Asn Leu Phe Arg Ala Ser Asp Leu Ala Phe Pro Asp Glu Arg Ala
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 Met Asp Asp Ala Arg Lys Phe Ala Glu Pro Tyr Leu Arg Glu Ala Leu
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 Ala Thr Lys Ile Ser Thr Asn Thr Lys Leu Phe Lys Glu Ile Glu Tyr
 485 490 495
 Val Val Glu Tyr Pro Trp His Met Ser Ile Pro Arg Leu Glu Ala Arg
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 Ser Tyr Ile Asp Ser Tyr Asp Asp Asn Tyr Val Trp Gln Arg Lys Thr
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 Thr Arg His Arg Val Ala Glu Val Tyr Phe Ser Ser Ala Thr Phe Glu
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 Pro Glu Tyr Ser Ala Thr Arg Ile Ala Phe Thr Lys Ile Gly Cys Leu
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 Gln Val Leu Phe Asp Asp Met Ala Asp Ile Phe Ala Thr Leu Asp Glu
 610 615 620
 Leu Lys Ser Phe Thr Glu Gly Val Lys Arg Trp Asp Thr Ser Leu Leu

| | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| 625 | | | | | 630 | | | | | 635 | | | | | 640 |
| His | Glu | Ile | Pro | Glu | Cys | Met | Gln | Thr | Cys | Phe | Lys | Val | Trp | Phe | Lys |
| | | | | 645 | | | | | 650 | | | | | 655 | |
| Leu | Met | Glu | Glu | Val | Asn | Asn | Asp | Val | Val | Lys | Val | Gln | Gly | Arg | Asp |
| | | | 660 | | | | | 665 | | | | | 670 | | |
| Met | Leu | Ala | His | Ile | Arg | Lys | Pro | Trp | Glu | Leu | Tyr | Phe | Asn | Cys | Tyr |
| | | 675 | | | | | 680 | | | | | 685 | | | |
| Val | Gln | Glu | Arg | Glu | Trp | Leu | Glu | Ala | Gly | Tyr | Ile | Pro | Thr | Phe | Glu |
| | 690 | | | | 695 | | | | | | 700 | | | | |
| Glu | Tyr | Leu | Lys | Thr | Tyr | Ala | Ile | Ser | Val | Gly | Leu | Gly | Pro | Cys | Thr |
| 705 | | | | | 710 | | | | | 715 | | | | | 720 |
| Leu | Gln | Pro | Ile | Leu | Leu | Met | Gly | Glu | Leu | Val | Lys | Asp | Asp | Val | Val |
| | | | 725 | | | | | | 730 | | | | | 735 | |
| Glu | Lys | Val | His | Tyr | Pro | Ser | Asn | Met | Phe | Glu | Leu | Val | Ser | Leu | Ser |
| | | | 740 | | | | | 745 | | | | | 750 | | |
| Trp | Arg | Leu | Thr | Asn | Asp | Thr | Lys | Thr | Tyr | Gln | Ala | Glu | Lys | Ala | Arg |
| | | 755 | | | | | 760 | | | | | 765 | | | |
| Gly | Gln | Gln | Ala | Ser | Gly | Ile | Ala | Cys | Tyr | Met | Lys | Asp | Asn | Pro | Gly |
| | 770 | | | | 775 | | | | | | 780 | | | | |
| Ala | Thr | Glu | Glu | Asp | Ala | Ile | Lys | His | Ile | Cys | Arg | Val | Val | Asp | Arg |
| 785 | | | | | 790 | | | | | 795 | | | | | 800 |
| Ala | Leu | Lys | Glu | Ala | Ser | Phe | Glu | Tyr | Phe | Lys | Pro | Ser | Asn | Asp | Ile |
| | | | | 805 | | | | | 810 | | | | | 815 | |
| Pro | Met | Gly | Cys | Lys | Ser | Phe | Ile | Phe | Asn | Leu | Arg | Leu | Cys | Val | Gln |
| | | | 820 | | | | | 825 | | | | | 830 | | |
| Ile | Phe | Tyr | Lys | Phe | Ile | Asp | Gly | Tyr | Gly | Ile | Ala | Asn | Glu | Glu | Ile |
| | 835 | | | | | 840 | | | | | | 845 | | | |
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<220>

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<223> E-alpha-bisabolene synthase

<400> 45

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| g | ggt | tat | gat | ctt | gtg | cat | tct | ctt | aaa | tca | cct | tat | att | gat | tct | agt | 49 |
| Gly | Tyr | Asp | Leu | Val | His | Ser | Leu | Lys | Ser | Pro | Tyr | Ile | Asp | Ser | Ser | | |
| 1 | | | | 5 | | | | | 10 | | | | | 15 | | | |
| tac | aga | gaa | cgc | gcg | gag | gtc | ctt | gtt | agc | gag | att | aaa | gtg | atg | ctt | | 97 |
| Tyr | Arg | Glu | Arg | Ala | Glu | Val | Leu | Val | Ser | Glu | Ile | Lys | Val | Met | Leu | | |
| | | | 20 | | | | 25 | | | | | | 30 | | | | |
| aat | cca | gct | att | aca | gga | gat | gga | gaa | tca | atg | att | act | cca | tct | gct | | 145 |
| Asn | Pro | Ala | Ile | Thr | Gly | Asp | Gly | Glu | Ser | Met | Ile | Thr | Pro | Ser | Ala | | |
| | | 35 | | | | 40 | | | | | | 45 | | | | | |

| | |
|---|-----|
| tat gac aca gca tgg gta gcg agg gtg ccc gcc att gat ggc tct gct | 193 |
| Tyr Asp Thr Ala Trp Val Ala Arg Val Pro Ala Ile Asp Gly Ser Ala | |
| 50 55 60 | |
| cgc ccg caa ttt ccc caa aca gtt gac tgg att ttg aaa aac cag tta | 241 |
| Arg Pro Gln Phe Pro Gln Thr Val Asp Trp Ile Leu Lys Asn Gln Leu | |
| 65 70 75 80 | |
| aaa gat ggt tca tgg gga att cag tcc cac ttt ctg ctg tcc gac cgt | 289 |
| Lys Asp Gly Ser Trp Gly Ile Gln Ser His Phe Leu Leu Ser Asp Arg | |
| 85 90 95 | |
| ctt ctt gcc act ctt tct tgt gtt ctt gtg ctc ctt aaa tgg aac gtt | 337 |
| Leu Leu Ala Thr Leu Ser Cys Val Leu Val Leu Leu Lys Trp Asn Val | |
| 100 105 110 | |
| ggg gat ctg caa gta gag cag gga att gaa ttc ata aag agc aat ctg | 385 |
| Gly Asp Leu Gln Val Glu Gln Gly Ile Glu Phe Ile Lys Ser Asn Leu | |
| 115 120 125 | |
| gaa cta gta aag gat gaa acc gat caa gat agc ttg gta aca gac ttt | 433 |
| Glu Leu Val Lys Asp Glu Thr Asp Gln Asp Ser Leu Val Thr Asp Phe | |
| 130 135 140 | |
| gag atc ata ttt cct tct ctg tta aga gaa gct caa tct ctg cgc ctc | 481 |
| Glu Ile Ile Phe Pro Ser Leu Leu Arg Glu Ala Gln Ser Leu Arg Leu | |
| 145 150 155 160 | |
| gga ctt ccc tac gac ctg cct tat ata cat ctg ttg cag act aaa cgg | 529 |
| Gly Leu Pro Tyr Asp Leu Pro Tyr Ile His Leu Leu Gln Thr Lys Arg | |
| 165 170 175 | |
| cag gaa aga tta gca aaa ctt tca agg gag gaa att tat gcg gtt ccg | 577 |
| Gln Glu Arg Leu Ala Lys Leu Ser Arg Glu Glu Ile Tyr Ala Val Pro | |
| 180 185 190 | |
| tcg cca ttg ttg tat tct tta gag gga ata caa gat ata gtt gaa tgg | 625 |
| Ser Pro Leu Leu Tyr Ser Leu Glu Gly Ile Gln Asp Ile Val Glu Trp | |
| 195 200 205 | |
| gaa cga ata atg gaa gtt caa agt cag gat ggg tct ttc tta agc tca | 673 |
| Glu Arg Ile Met Glu Val Gln Ser Gln Asp Gly Ser Phe Leu Ser Ser | |
| 210 215 220 | |
| cct gct tct act gcc tgc gtt ttc atg cac aca gga gac gcg aaa tgc | 721 |
| Pro Ala Ser Thr Ala Cys Val Phe Met His Thr Gly Asp Ala Lys Cys | |
| 225 230 235 240 | |
| ctt gaa ttc ttg aac agt gtg atg atc aag ttt gga aat ttt gtt ccc | 769 |
| Leu Glu Phe Leu Asn Ser Val Met Ile Lys Phe Gly Asn Phe Val Pro | |
| 245 250 255 | |
| tgc ctg tat cct gtg gat ctg ctg gaa cgc ctg ttg atc gta gat aat | 817 |

| | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|
| Cys | Leu | Tyr | Pro | Val | Asp | Leu | Leu | Glu | Arg | Leu | Leu | Ile | Val | Asp | Asn | |
| | | | 260 | | | | | 265 | | | | | 270 | | | |
| att | gta | cgc | ctt | gga | atc | tat | aga | cac | ttt | gaa | aag | gaa | atc | aag | gaa | 865 |
| Ile | Val | Arg | Leu | Gly | Ile | Tyr | Arg | His | Phe | Glu | Lys | Glu | Ile | Lys | Glu | |
| | | 275 | | | | | 280 | | | | | 285 | | | | |
| gct | ctt | gat | tat | gtt | tac | agg | cat | tgg | aac | gaa | aga | gga | att | ggg | tgg | 913 |
| Ala | Leu | Asp | Tyr | Val | Tyr | Arg | His | Trp | Asn | Glu | Arg | Gly | Ile | Gly | Trp | |
| | 290 | | | | | 295 | | | | | 300 | | | | | |
| ggc | aga | cta | aat | ccc | ata | gca | gat | ctt | gag | acc | act | gct | ttg | gga | ttt | 961 |
| Gly | Arg | Leu | Asn | Pro | Ile | Ala | Asp | Leu | Glu | Thr | Thr | Ala | Leu | Gly | Phe | |
| 305 | | | | | 310 | | | | | 315 | | | | | 320 | |
| cga | ttg | ctt | cgg | ctg | cat | agg | tac | aat | gta | tct | cca | gcc | att | ttt | gac | 1009 |
| Arg | Leu | Leu | Arg | Leu | His | Arg | Tyr | Asn | Val | Ser | Pro | Ala | Ile | Phe | Asp | |
| | | | | 325 | | | | | 330 | | | | | 335 | | |
| aac | ttc | aaa | gat | gcc | aat | ggg | aaa | ttc | att | tgc | tcg | acc | ggg | caa | ttc | 1057 |
| Asn | Phe | Lys | Asp | Ala | Asn | Gly | Lys | Phe | Ile | Cys | Ser | Thr | Gly | Gln | Phe | |
| | | | 340 | | | | | 345 | | | | | 350 | | | |
| aac | aaa | gat | gta | gca | agc | atg | ctg | aat | ctt | tat | aga | gct | tcc | cag | ctc | 1105 |
| Asn | Lys | Asp | Val | Ala | Ser | Met | Leu | Asn | Leu | Tyr | Arg | Ala | Ser | Gln | Leu | |
| | | 355 | | | | | 360 | | | | | 365 | | | | |
| gca | ttt | ccc | gga | gaa | aac | att | ctt | gat | gaa | gct | aaa | agc | ttc | gct | act | 1153 |
| Ala | Phe | Pro | Gly | Glu | Asn | Ile | Leu | Asp | Glu | Ala | Lys | Ser | Phe | Ala | Thr | |
| | 370 | | | | | 375 | | | | | 380 | | | | | |
| aaa | tat | ttg | aga | gaa | gct | ctt | gag | aaa | agt | gag | act | tcc | agt | gca | tgg | 1201 |
| Lys | Tyr | Leu | Arg | Glu | Ala | Leu | Glu | Lys | Ser | Glu | Thr | Ser | Ser | Ala | Trp | |
| 385 | | | | | 390 | | | | | 395 | | | | | 400 | |
| aac | aac | aaa | caa | aac | ctg | agc | caa | gag | atc | aaa | tac | gcg | ctg | aag | act | 1249 |
| Asn | Asn | Lys | Gln | Asn | Leu | Ser | Gln | Glu | Ile | Lys | Tyr | Ala | Leu | Lys | Thr | |
| | | | | 405 | | | | | 410 | | | | | 415 | | |
| tct | tgg | cat | gcc | agt | gtt | ccg | aga | gtg | gaa | gca | aag | aga | tac | tgt | caa | 1297 |
| Ser | Trp | His | Ala | Ser | Val | Pro | Arg | Val | Glu | Ala | Lys | Arg | Tyr | Cys | Gln | |
| | | | 420 | | | | | 425 | | | | | 430 | | | |
| gtg | tat | cgc | cca | gat | tat | gca | cgc | ata | gca | aaa | tgc | gtt | tac | aag | cta | 1345 |
| Val | Tyr | Arg | Pro | Asp | Tyr | Ala | Arg | Ile | Ala | Lys | Cys | Val | Tyr | Lys | Leu | |
| | | 435 | | | | | 440 | | | | | 445 | | | | |
| ccc | tac | gtg | aac | aat | gaa | aag | ttt | tta | gag | ctg | gga | aaa | tta | gat | ttc | 1393 |
| Pro | Tyr | Val | Asn | Asn | Glu | Lys | Phe | Leu | Glu | Leu | Gly | Lys | Leu | Asp | Phe | |
| | 450 | | | | | 455 | | | | | 460 | | | | | |
| aac | att | atc | cag | tcc | atc | cac | caa | gaa | gaa | atg | aag | aat | gtt | acc | agc | 1441 |
| Asn | Ile | Ile | Gln | Ser | Ile | His | Gln | Glu | Glu | Met | Lys | Asn | Val | Thr | Ser | |

| 465 | 470 | 475 | 480 | |
|---|-----|-----|-----|------|
| tgg ttt aga gat tgc ggg ttg cca cta ttc acc ttc gct cgg gag agg | 485 | 490 | 495 | 1489 |
| Trp Phe Arg Asp Ser Gly Leu Pro Leu Phe Thr Phe Ala Arg Glu Arg | | | | |
| ccg ctg gaa ttc tac ttc tta gta gcg gcg ggg acc tat gaa ccc cag | 500 | 505 | 510 | 1537 |
| Pro Leu Glu Phe Tyr Phe Leu Val Ala Ala Gly Thr Tyr Glu Pro Gln | | | | |
| tat gcc aaa tgc agg ttc ctc ttt aca aaa gtg gca tgc ttg cag act | 515 | 520 | 525 | 1585 |
| Tyr Ala Lys Cys Arg Phe Leu Phe Thr Lys Val Ala Cys Leu Gln Thr | | | | |
| gtt ctg gac gat atg tat gac act tat gga acc cta gat gaa ttg aag | 530 | 535 | 540 | 1633 |
| Val Leu Asp Asp Met Tyr Asp Thr Tyr Gly Thr Leu Asp Glu Leu Lys | | | | |
| cta ttc act gag gct gtg aga aga tgg gac ctc tcc ttt aca gaa aac | 545 | 550 | 555 | 1681 |
| Leu Phe Thr Glu Ala Val Arg Arg Trp Asp Leu Ser Phe Thr Glu Asn | | | | |
| ctt cca gac tat atg aaa cta tgt tac caa atc tat tat gac ata gtt | 565 | 570 | 575 | 1729 |
| Leu Pro Asp Tyr Met Lys Leu Cys Tyr Gln Ile Tyr Tyr Asp Ile Val | | | | |
| cac gag gtg gct tgg gag gca gag aag gaa cag ggg cgt gaa ttg gtc | 580 | 585 | 590 | 1777 |
| His Glu Val Ala Trp Glu Ala Glu Lys Glu Gln Gly Arg Glu Leu Val | | | | |
| agc ttt ttc aga aag gga tgg gag gat tat ctt ctg ggt tat tat gaa | 595 | 600 | 605 | 1825 |
| Ser Phe Phe Arg Lys Gly Trp Glu Asp Tyr Leu Leu Gly Tyr Tyr Glu | | | | |
| gaa gct gaa tgg tta gct gct gag tat gtg cct acc ttg gac gag tac | 610 | 615 | 620 | 1873 |
| Glu Ala Glu Trp Leu Ala Ala Glu Tyr Val Pro Thr Leu Asp Glu Tyr | | | | |
| ata aag aat gga atc aca tct atc ggc caa cgt ata ctt ctg ttg agt | 625 | 630 | 635 | 1921 |
| Ile Lys Asn Gly Ile Thr Ser Ile Gly Gln Arg Ile Leu Leu Leu Ser | | | | |
| gga gtg ttg ata atg gat ggg caa ctc ctt tgc caa gag gca tta gag | 645 | 650 | 655 | 1969 |
| Gly Val Leu Ile Met Asp Gly Gln Leu Leu Ser Gln Glu Ala Leu Glu | | | | |
| aaa gta gat tat cca gga aga cgt gtt ctc aca gag ctg aat agc ctc | 660 | 665 | 670 | 2017 |
| Lys Val Asp Tyr Pro Gly Arg Arg Val Leu Thr Glu Leu Asn Ser Leu | | | | |
| att tcc cgc ctg gcg gat gac acg aag aca tat aaa gct gag aag gct | 675 | 680 | 685 | 2065 |
| Ile Ser Arg Leu Ala Asp Asp Thr Lys Thr Tyr Lys Ala Glu Lys Ala | | | | |


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cgt gga gaa ttg gcg tcc agc att gaa tgt tac atg aaa gac cat cct      2113
Arg Gly Glu Leu Ala Ser Ser Ile Glu Cys Tyr Met Lys Asp His Pro
690                               695                               700

gaa tgt aca gag gaa gag gct ctc gat cac atc tat agc att ctg gag      2161
Glu Cys Thr Glu Glu Glu Ala Leu Asp His Ile Tyr Ser Ile Leu Glu
705                               710                               715                               720

ccg gcg gtg aag gaa ctg aca aga gag ttt ctg aag ccc gac gac gtc      2209
Pro Ala Val Lys Glu Leu Thr Arg Glu Phe Leu Lys Pro Asp Asp Val
725                               730                               735

cca ttc gcc tgc aag aag atg ctt ttc gag gag aca aga gtg acg atg      2257
Pro Phe Ala Cys Lys Lys Met Leu Phe Glu Glu Thr Arg Val Thr Met
740                               745                               750

gtg ata ttc aag gat gga gat gga ttc ggt gtt tcc aaa tta gaa gtc      2305
Val Ile Phe Lys Asp Gly Asp Gly Phe Gly Val Ser Lys Leu Glu Val
755                               760                               765

aaa gat cat atc aaa gag tgt ctc att gaa ccg ctg cca ctg taa      2350
Lys Asp His Ile Lys Glu Cys Leu Ile Glu Pro Leu Pro Leu *
770                               775                               780

tcaaaatagt tgcaataata attgaaataa tgtcaactat gtttcacaaa aaaaaaaaaa 2410
aaaaaaaaaa aaaa                                     2424

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<211> 782
<212> PRT
<213> Abies grandis

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Asn Pro Ala Ile Thr Gly Asp Gly Glu Ser Met Ile Thr Pro Ser Ala
35      40      45
Tyr Asp Thr Ala Trp Val Ala Arg Val Pro Ala Ile Asp Gly Ser Ala
50      55      60
Arg Pro Gln Phe Pro Gln Thr Val Asp Trp Ile Leu Lys Asn Gln Leu
65      70      75      80
Lys Asp Gly Ser Trp Gly Ile Gln Ser His Phe Leu Leu Ser Asp Arg
85      90      95
Leu Leu Ala Thr Leu Ser Cys Val Leu Val Leu Leu Lys Trp Asn Val
100     105     110
Gly Asp Leu Gln Val Glu Gln Gly Ile Glu Phe Ile Lys Ser Asn Leu
115     120     125
Glu Leu Val Lys Asp Glu Thr Asp Gln Asp Ser Leu Val Thr Asp Phe
130     135     140
Glu Ile Ile Phe Pro Ser Leu Leu Arg Glu Ala Gln Ser Leu Arg Leu

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| | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| 145 | | | | | 150 | | | | | 155 | | | | | 160 |
| Gly | Leu | Pro | Tyr | Asp | Leu | Pro | Tyr | Ile | His | Leu | Leu | Gln | Thr | Lys | Arg |
| | | | | 165 | | | | | 170 | | | | | 175 | |
| Gln | Glu | Arg | Leu | Ala | Lys | Leu | Ser | Arg | Glu | Glu | Ile | Tyr | Ala | Val | Pro |
| | | | | 180 | | | | | 185 | | | | | 190 | |
| Ser | Pro | Leu | Leu | Tyr | Ser | Leu | Glu | Gly | Ile | Gln | Asp | Ile | Val | Glu | Trp |
| | | | | 195 | | | | | 200 | | | | | 205 | |
| Glu | Arg | Ile | Met | Glu | Val | Gln | Ser | Gln | Asp | Gly | Ser | Phe | Leu | Ser | Ser |
| | | | | 210 | | | | | 215 | | | | | 220 | |
| Pro | Ala | Ser | Thr | Ala | Cys | Val | Phe | Met | His | Thr | Gly | Asp | Ala | Lys | Cys |
| | | | | 225 | | | | | 230 | | | | | 235 | |
| Leu | Glu | Phe | Leu | Asn | Ser | Val | Met | Ile | Lys | Phe | Gly | Asn | Phe | Val | Pro |
| | | | | 245 | | | | | 250 | | | | | 255 | |
| Cys | Leu | Tyr | Pro | Val | Asp | Leu | Leu | Glu | Arg | Leu | Leu | Ile | Val | Asp | Asn |
| | | | | 260 | | | | | 265 | | | | | 270 | |
| Ile | Val | Arg | Leu | Gly | Ile | Tyr | Arg | His | Phe | Glu | Lys | Glu | Ile | Lys | Glu |
| | | | | 275 | | | | | 280 | | | | | 285 | |
| Ala | Leu | Asp | Tyr | Val | Tyr | Arg | His | Trp | Asn | Glu | Arg | Gly | Ile | Gly | Trp |
| | | | | 290 | | | | | 295 | | | | | 300 | |
| Gly | Arg | Leu | Asn | Pro | Ile | Ala | Asp | Leu | Glu | Thr | Thr | Ala | Leu | Gly | Phe |
| | | | | 305 | | | | | 310 | | | | | 315 | |
| Arg | Leu | Leu | Arg | Leu | His | Arg | Tyr | Asn | Val | Ser | Pro | Ala | Ile | Phe | Asp |
| | | | | 325 | | | | | 330 | | | | | 335 | |
| Asn | Phe | Lys | Asp | Ala | Asn | Gly | Lys | Phe | Ile | Cys | Ser | Thr | Gly | Gln | Phe |
| | | | | 340 | | | | | 345 | | | | | 350 | |
| Asn | Lys | Asp | Val | Ala | Ser | Met | Leu | Asn | Leu | Tyr | Arg | Ala | Ser | Gln | Leu |
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| Ala | Phe | Pro | Gly | Glu | Asn | Ile | Leu | Asp | Glu | Ala | Lys | Ser | Phe | Ala | Thr |
| | | | | 370 | | | | | 375 | | | | | 380 | |
| Lys | Tyr | Leu | Arg | Glu | Ala | Leu | Glu | Lys | Ser | Glu | Thr | Ser | Ser | Ala | Trp |
| | | | | 385 | | | | | 390 | | | | | 395 | |
| Asn | Asn | Lys | Gln | Asn | Leu | Ser | Gln | Glu | Ile | Lys | Tyr | Ala | Leu | Lys | Thr |
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| Ser | Trp | His | Ala | Ser | Val | Pro | Arg | Val | Glu | Ala | Lys | Arg | Tyr | Cys | Gln |
| | | | | 420 | | | | | 425 | | | | | 430 | |
| Val | Tyr | Arg | Pro | Asp | Tyr | Ala | Arg | Ile | Ala | Lys | Cys | Val | Tyr | Lys | Leu |
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| Pro | Tyr | Val | Asn | Asn | Glu | Lys | Phe | Leu | Glu | Leu | Gly | Lys | Leu | Asp | Phe |
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| Asn | Ile | Ile | Gln | Ser | Ile | His | Gln | Glu | Glu | Met | Lys | Asn | Val | Thr | Ser |
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| Trp | Phe | Arg | Asp | Ser | Gly | Leu | Pro | Leu | Phe | Thr | Phe | Ala | Arg | Glu | Arg |
| | | | | 485 | | | | | 490 | | | | | 495 | |
| Pro | Leu | Glu | Phe | Tyr | Phe | Leu | Val | Ala | Ala | Gly | Thr | Tyr | Glu | Pro | Gln |
| | | | | 500 | | | | | 505 | | | | | 510 | |
| Tyr | Ala | Lys | Cys | Arg | Phe | Leu | Phe | Thr | Lys | Val | Ala | Cys | Leu | Gln | Thr |
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| Val | Leu | Asp | Asp | Met | Tyr | Asp | Thr | Tyr | Gly | Thr | Leu | Asp | Glu | Leu | Lys |
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| Leu | Phe | Thr | Glu | Ala | Val | Arg | Arg | Trp | Asp | Leu | Ser | Phe | Thr | Glu | Asn |
| | | | | 545 | | | | | 550 | | | | | 555 | |
| Leu | Pro | Asp | Tyr | Met | Lys | Leu | Cys | Tyr | Gln | Ile | Tyr | Tyr | Asp | Ile | Val |
| | | | | 565 | | | | | 570 | | | | | 575 | |

His Glu Val Ala Trp Glu Ala Glu Lys Glu Gln Gly Arg Glu Leu Val
 580 585 590
 Ser Phe Phe Arg Lys Gly Trp Glu Asp Tyr Leu Leu Gly Tyr Tyr Glu
 595 600 605
 Glu Ala Glu Trp Leu Ala Ala Glu Tyr Val Pro Thr Leu Asp Glu Tyr
 610 615 620
 Ile Lys Asn Gly Ile Thr Ser Ile Gly Gln Arg Ile Leu Leu Leu Ser
 625 630 635
 Gly Val Leu Ile Met Asp Gly Gln Leu Leu Ser Gln Glu Ala Leu Glu
 645 650 655
 Lys Val Asp Tyr Pro Gly Arg Arg Val Leu Thr Glu Leu Asn Ser Leu
 660 665 670
 Ile Ser Arg Leu Ala Asp Asp Thr Lys Thr Tyr Lys Ala Glu Lys Ala
 675 680 685
 Arg Gly Glu Leu Ala Ser Ser Ile Glu Cys Tyr Met Lys Asp His Pro
 690 695 700
 Glu Cys Thr Glu Glu Glu Ala Leu Asp His Ile Tyr Ser Ile Leu Glu
 705 710 715 720
 Pro Ala Val Lys Glu Leu Thr Arg Glu Phe Leu Lys Pro Asp Asp Val
 725 730 735
 Pro Phe Ala Cys Lys Lys Met Leu Phe Glu Glu Thr Arg Val Thr Met
 740 745 750
 Val Ile Phe Lys Asp Gly Asp Gly Phe Gly Val Ser Lys Leu Glu Val
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<211> 1865

<212> DNA

<213> Abies grandis

<220>

<221> CDS

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<223> d-selinene synthase

<400> 47

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| Met Ala Glu Ile Ser Glu Ser Ser Ile Pro Arg Arg Thr Gly Asn His | |
| 1 5 10 15 | |
| cac gga aat gtg tgg gac gat gac ctc ata cac tct ctc aac tcg ccc | 96 |
| His Gly Asn Val Trp Asp Asp Asp Leu Ile His Ser Leu Asn Ser Pro | |
| 20 25 30 | |
| tat ggg gca cct gca tat tat gag ctc ctt caa aag ctt att cag gag | 144 |
| Tyr Gly Ala Pro Ala Tyr Tyr Glu Leu Leu Gln Lys Leu Ile Gln Glu | |
| 35 40 45 | |
| atc aag cat tta ctt ttg act gaa atg gaa atg gat gat ggc gat cat | 192 |
| Ile Lys His Leu Leu Leu Thr Glu Met Glu Met Asp Asp Gly Asp His | |
| 50 55 60 | |

| | |
|---|-----|
| gat tta atc aaa cgt ctt cag atc gtt gac act ttg gaa tgc ctg gga Asp Leu Ile Lys Arg Leu Gln Ile Val Asp Thr Leu Glu Cys Leu Gly 65 70 75 80 | 240 |
| atc gat aga cat ttt gaa cac gaa ata caa aca gct gct tta gat tac Ile Asp Arg His Phe Glu His Glu Ile Gln Thr Ala Ala Leu Asp Tyr 85 90 95 | 288 |
| gtt tac aga tgg tgg aac gaa aaa ggt atc ggg gag gga tca aga gat Val Tyr Arg Trp Trp Asn Glu Lys Gly Ile Gly Glu Gly Ser Arg Asp 100 105 110 | 336 |
| tcc ttc agc aaa gat ctg aac gct acg gct tta gga ttt cgc gct ctc Ser Phe Ser Lys Asp Leu Asn Ala Thr Ala Leu Gly Phe Arg Ala Leu 115 120 125 | 384 |
| cga ctg cat cga tat aac gta tcg tca ggt gtg ttg aag aat ttc aag Arg Leu His Arg Tyr Asn Val Ser Ser Gly Val Leu Lys Asn Phe Lys 130 135 140 | 432 |
| gat gaa aac ggg aag ttc ttc tgc aac ttt act ggt gaa gaa gga aga Asp Glu Asn Gly Lys Phe Phe Cys Asn Phe Thr Gly Glu Glu Gly Arg 145 150 155 160 | 480 |
| gga gat aaa caa gtg aga agc atg ttg tcg tta ctt cga gct tca gag Gly Asp Lys Gln Val Arg Ser Met Leu Ser Leu Leu Arg Ala Ser Glu 165 170 175 | 528 |
| att tcg ttt ccc gga gaa aaa gtg atg gaa gag gcc aag gca ttc aca Ile Ser Phe Pro Gly Glu Lys Val Met Glu Glu Ala Lys Ala Phe Thr 180 185 190 | 576 |
| aga gaa tat cta aac caa gtt tta gct gga cac ggg gat gtg act gac Arg Glu Tyr Leu Asn Gln Val Leu Ala Gly His Gly Asp Val Thr Asp 195 200 205 | 624 |
| gtg gat caa agc ctt ttg aga gag gtg aag tac gca ttg gag ttt cca Val Asp Gln Ser Leu Leu Arg Glu Val Lys Tyr Ala Leu Glu Phe Pro 210 215 220 | 672 |
| tgg cat tgc agt gtg ccg aga tgg gag gca agg agc ttt ctc gaa ata Trp His Cys Ser Val Pro Arg Trp Glu Ala Arg Ser Phe Leu Glu Ile 225 230 235 240 | 720 |
| tat gga cac aac cat tcg tgg ctc aag tcg aat atc aac caa aaa atg Tyr Gly His Asn His Ser Trp Leu Lys Ser Asn Ile Asn Gln Lys Met 245 250 255 | 768 |
| ttg aag tta gcc aaa ttg gac ttc aat att ctg caa tgc aaa cat cac Leu Lys Leu Ala Lys Leu Asp Phe Asn Ile Leu Gln Cys Lys His His 260 265 270 | 816 |

| | |
|---|------|
| aag gag ata cag ttt att aca agg tgg tgg aga gac tcg ggt ata tcg Lys Glu Ile Gln Phe Ile Thr Arg Trp Trp Arg Asp Ser Gly Ile Ser 275 280 285 | 864 |
| cag ctg aat ttc tat cga aag cga cac gtg gaa tat tat tct tgg gtt Gln Leu Asn Phe Tyr Arg Lys Arg His Val Glu Tyr Tyr Ser Trp Val 290 295 300 | 912 |
| gtt atg tgc att ttt gag cca gag ttc tct gaa agt aga att gcc ttc Val Met Cys Ile Phe Glu Pro Glu Phe Ser Glu Ser Arg Ile Ala Phe 305 310 315 320 | 960 |
| gcc aaa act gct atc ctg tgt act gtt cta gat gac ctc tat gat acg Ala Lys Thr Ala Ile Leu Cys Thr Val Leu Asp Asp Leu Tyr Asp Thr 325 330 335 | 1008 |
| cac gca aca ttg cat gaa atc aaa atc atg aca gag gga gtg aga cga His Ala Thr Leu His Glu Ile Lys Ile Met Thr Glu Gly Val Arg Arg 340 345 350 | 1056 |
| tgg gat ctt tcg ttg aca gat gac ctc cca gac tac att aaa att gca Trp Asp Leu Ser Leu Thr Asp Asp Leu Pro Asp Tyr Ile Lys Ile Ala 355 360 365 | 1104 |
| ttc cag ttc ttc ttc aat aca gtg aat gaa ttg ata gtt gaa atc gtg Phe Gln Phe Phe Phe Asn Thr Val Asn Glu Leu Ile Val Glu Ile Val 370 375 380 | 1152 |
| aaa cgg caa ggg cgg gat atg aca acc ata gtt aaa gat tgc tgg aag Lys Arg Gln Gly Arg Asp Met Thr Thr Ile Val Lys Asp Cys Trp Lys 385 390 395 400 | 1200 |
| cga tac att gag tct tat ctg caa gaa gcg gaa tgg ata gca act gga Arg Tyr Ile Glu Ser Tyr Leu Gln Glu Ala Glu Trp Ile Ala Thr Gly 405 410 415 | 1248 |
| cat att ccc act ttt aac gaa tac ata aag aac ggc atg gct agc tca His Ile Pro Thr Phe Asn Glu Tyr Ile Lys Asn Gly Met Ala Ser Ser 420 425 430 | 1296 |
| ggg atg tgt att cta aat ttg aat cca ctt ctc ttg ttg gat aaa ctt Gly Met Cys Ile Leu Asn Leu Asn Pro Leu Leu Leu Leu Asp Lys Leu 435 440 445 | 1344 |
| ctc ccc gac aac att ctg gag caa ata cat tct cca tcc aag atc ctg Leu Pro Asp Asn Ile Leu Glu Gln Ile His Ser Pro Ser Lys Ile Leu 450 455 460 | 1392 |
| gac ctc tta gaa ttg acg ggc aga atc gcc gat gac tta aaa gat ttc Asp Leu Leu Glu Leu Thr Gly Arg Ile Ala Asp Asp Leu Lys Asp Phe 465 470 475 480 | 1440 |
| gag gac gag aag gaa cgc ggg gag atg gct tca tct tta cag tgt tat | 1488 |

| | | | | | | | | | | | | | | | | |
|------------|------------|------------|------------|-------------|------------|-------------|------------|------------|-----|-----|-----|-----|-----|-----|-----|------|
| Glu | Asp | Glu | Lys | Glu | Arg | Gly | Glu | Met | Ala | Ser | Ser | Leu | Gln | Cys | Tyr | |
| | | | | 485 | | | | | 490 | | | | | 495 | | |
| atg | aaa | gaa | aat | cct | gaa | tct | aca | gtg | gaa | aat | gct | tta | aat | cac | ata | 1536 |
| Met | Lys | Glu | Asn | Pro | Glu | Ser | Thr | Val | Glu | Asn | Ala | Leu | Asn | His | Ile | |
| | | | 500 | | | | | 505 | | | | | 510 | | | |
| aaa | ggc | atc | ctt | aat | cgt | tcc | ctt | gag | gaa | ttt | aat | tgg | gag | ttt | atg | 1584 |
| Lys | Gly | Ile | Leu | Asn | Arg | Ser | Leu | Glu | Glu | Phe | Asn | Trp | Glu | Phe | Met | |
| | | 515 | | | | | 520 | | | | | 525 | | | | |
| aag | cag | gat | agt | gtc | cca | atg | tgt | tgc | aag | aaa | ttc | act | ttc | aat | ata | 1632 |
| Lys | Gln | Asp | Ser | Val | Pro | Met | Cys | Cys | Lys | Lys | Phe | Thr | Phe | Asn | Ile | |
| | 530 | | | | | 535 | | | | | 540 | | | | | |
| ggg | cga | gga | ctt | caa | ttc | atc | tac | aaa | tac | aga | gac | ggc | tta | tac | att | 1680 |
| Gly | Arg | Gly | Leu | Gln | Phe | Ile | Tyr | Lys | Tyr | Arg | Asp | Gly | Leu | Tyr | Ile | |
| 545 | | | | 550 | | | | | 555 | | | | | | 560 | |
| tct | gac | aag | gaa | gta | aag | gac | cag | ata | ttc | aaa | att | cta | gtc | cac | caa | 1728 |
| Ser | Asp | Lys | Glu | Val | Lys | Asp | Gln | Ile | Phe | Lys | Ile | Leu | Val | His | Gln | |
| | | | | 565 | | | | | 570 | | | | | 575 | | |
| gtt | cca | atg | gag | gaa | tag | tgatgggtctt | gggtgtagtt | gtctattatg | | | | | | | | 1776 |
| Val | Pro | Met | Glu | Glu | * | | | | | | | | | | | |
| | | | 580 | | | | | | | | | | | | | |
| gtatattgca | ttgacattta | tgcttaaagg | tgtttcttaa | acgttttaggg | cggaccgcta | | | | | | | | | | | 1836 |
| aataagttgg | caataattaa | tatctcgag | | | | | | | | | | | | | | 1865 |

<210> 48
 <211> 581
 <212> PRT
 <213> Abies grandis

| | | | | | | | | | | | | | | | |
|----------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| <400> 48 | | | | | | | | | | | | | | | |
| Met | Ala | Glu | Ile | Ser | Glu | Ser | Ser | Ile | Pro | Arg | Arg | Thr | Gly | Asn | His |
| 1 | | | | 5 | | | | | 10 | | | | | 15 | |
| His | Gly | Asn | Val | Trp | Asp | Asp | Asp | Leu | Ile | His | Ser | Leu | Asn | Ser | Pro |
| | | | 20 | | | | | 25 | | | | | 30 | | |
| Tyr | Gly | Ala | Pro | Ala | Tyr | Tyr | Glu | Leu | Leu | Gln | Lys | Leu | Ile | Gln | Glu |
| | | 35 | | | | | 40 | | | | | 45 | | | |
| Ile | Lys | His | Leu | Leu | Leu | Thr | Glu | Met | Glu | Met | Asp | Asp | Gly | Asp | His |
| | 50 | | | | | 55 | | | | | 60 | | | | |
| Asp | Leu | Ile | Lys | Arg | Leu | Gln | Ile | Val | Asp | Thr | Leu | Glu | Cys | Leu | Gly |
| 65 | | | | | 70 | | | | 75 | | | | | 80 | |
| Ile | Asp | Arg | His | Phe | Glu | His | Glu | Ile | Gln | Thr | Ala | Ala | Leu | Asp | Tyr |
| | | | 85 | | | | | | 90 | | | | | 95 | |
| Val | Tyr | Arg | Trp | Trp | Asn | Glu | Lys | Gly | Ile | Gly | Glu | Gly | Ser | Arg | Asp |
| | | | 100 | | | | | 105 | | | | | 110 | | |
| Ser | Phe | Ser | Lys | Asp | Leu | Asn | Ala | Thr | Ala | Leu | Gly | Phe | Arg | Ala | Leu |
| | | 115 | | | | | 120 | | | | | 125 | | | |
| Arg | Leu | His | Arg | Tyr | Asn | Val | Ser | Ser | Gly | Val | Leu | Lys | Asn | Phe | Lys |

| | | |
|---|-----|-----|
| 130 | 135 | 140 |
| Asp Glu Asn Gly Lys Phe Phe Cys Asn Phe Thr Gly Glu Glu Gly Arg | | |
| 145 | 150 | 155 |
| Gly Asp Lys Gln Val Arg Ser Met Leu Ser Leu Leu Arg Ala Ser Glu | | |
| | 165 | 170 |
| Ile Ser Phe Pro Gly Glu Lys Val Met Glu Glu Ala Lys Ala Phe Thr | | |
| | 180 | 185 |
| Arg Glu Tyr Leu Asn Gln Val Leu Ala Gly His Gly Asp Val Thr Asp | | |
| | 195 | 200 |
| Val Asp Gln Ser Leu Leu Arg Glu Val Lys Tyr Ala Leu Glu Phe Pro | | |
| | 210 | 215 |
| Trp His Cys Ser Val Pro Arg Trp Glu Ala Arg Ser Phe Leu Glu Ile | | |
| 225 | 230 | 235 |
| Tyr Gly His Asn His Ser Trp Leu Lys Ser Asn Ile Asn Gln Lys Met | | |
| | 245 | 250 |
| Leu Lys Leu Ala Lys Leu Asp Phe Asn Ile Leu Gln Cys Lys His His | | |
| | 260 | 265 |
| Lys Glu Ile Gln Phe Ile Thr Arg Trp Trp Arg Asp Ser Gly Ile Ser | | |
| | 275 | 280 |
| Gln Leu Asn Phe Tyr Arg Lys Arg His Val Glu Tyr Tyr Ser Trp Val | | |
| | 290 | 295 |
| Val Met Cys Ile Phe Glu Pro Glu Phe Ser Glu Ser Arg Ile Ala Phe | | |
| 305 | 310 | 315 |
| Ala Lys Thr Ala Ile Leu Cys Thr Val Leu Asp Asp Leu Tyr Asp Thr | | |
| | 325 | 330 |
| His Ala Thr Leu His Glu Ile Lys Ile Met Thr Glu Gly Val Arg Arg | | |
| | 340 | 345 |
| Trp Asp Leu Ser Leu Thr Asp Asp Leu Pro Asp Tyr Ile Lys Ile Ala | | |
| | 355 | 360 |
| Phe Gln Phe Phe Phe Asn Thr Val Asn Glu Leu Ile Val Glu Ile Val | | |
| | 370 | 375 |
| Lys Arg Gln Gly Arg Asp Met Thr Thr Ile Val Lys Asp Cys Trp Lys | | |
| 385 | 390 | 395 |
| Arg Tyr Ile Glu Ser Tyr Leu Gln Glu Ala Glu Trp Ile Ala Thr Gly | | |
| | 405 | 410 |
| His Ile Pro Thr Phe Asn Glu Tyr Ile Lys Asn Gly Met Ala Ser Ser | | |
| | 420 | 425 |
| Gly Met Cys Ile Leu Asn Leu Asn Pro Leu Leu Leu Leu Asp Lys Leu | | |
| | 435 | 440 |
| Leu Pro Asp Asn Ile Leu Glu Gln Ile His Ser Pro Ser Lys Ile Leu | | |
| | 450 | 455 |
| Asp Leu Leu Glu Leu Thr Gly Arg Ile Ala Asp Asp Leu Lys Asp Phe | | |
| 465 | 470 | 475 |
| Glu Asp Glu Lys Glu Arg Gly Glu Met Ala Ser Ser Leu Gln Cys Tyr | | |
| | 485 | 490 |
| Met Lys Glu Asn Pro Glu Ser Thr Val Glu Asn Ala Leu Asn His Ile | | |
| | 500 | 505 |
| Lys Gly Ile Leu Asn Arg Ser Leu Glu Glu Phe Asn Trp Glu Phe Met | | |
| | 515 | 520 |
| Lys Gln Asp Ser Val Pro Met Cys Cys Lys Lys Phe Thr Phe Asn Ile | | |
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| Gly Arg Gly Leu Gln Phe Ile Tyr Lys Tyr Arg Asp Gly Leu Tyr Ile | | |
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<222> (4)...(1785)
<223> gamma-humulene synthase
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90

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| Asn | Val | Ser | Ser | Gly | Val | Leu | Glu | Asn | Phe | Arg | Asp | Asp | Asn | Gly | Gln | | |
| 145 | | | | | | 150 | | | | | 155 | | | | | | |
| ttc | ttc | tgc | ggt | tct | aca | gtt | gaa | gaa | gaa | gga | gca | gaa | gca | tat | aat | 528 | |
| Phe | Phe | Cys | Gly | Ser | Thr | Val | Glu | Glu | Glu | Gly | Ala | Glu | Ala | Tyr | Asn | | |
| 160 | | | | | 165 | | | | | 170 | | | | | 175 | | |
| aaa | cac | gta | aga | tgc | atg | ctg | tca | tta | tcg | cga | gct | tca | aac | att | tta | 576 | |
| Lys | His | Val | Arg | Cys | Met | Leu | Ser | Leu | Ser | Arg | Ala | Ser | Asn | Ile | Leu | | |
| | | | | 180 | | | | | 185 | | | | | 190 | | | |
| ttt | ccg | ggc | gaa | aaa | gtg | atg | gaa | gag | gcg | aag | gca | ttc | aca | aca | aat | 624 | |
| Phe | Pro | Gly | Glu | Lys | Val | Met | Glu | Glu | Ala | Lys | Ala | Phe | Thr | Thr | Asn | | |
| | | | 195 | | | | | 200 | | | | | 205 | | | | |
| tat | cta | aag | aaa | gtt | tta | gca | gga | cgg | gag | gct | acc | cac | gtc | gat | gaa | 672 | |
| Tyr | Leu | Lys | Lys | Val | Leu | Ala | Gly | Arg | Glu | Ala | Thr | His | Val | Asp | Glu | | |
| | | 210 | | | | | 215 | | | | | 220 | | | | | |
| agc | ctt | ttg | gga | gag | gtg | aag | tac | gca | ttg | gag | ttt | cca | tgg | cat | tgc | 720 | |
| Ser | Leu | Leu | Gly | Glu | Val | Lys | Tyr | Ala | Leu | Glu | Phe | Pro | Trp | His | Cys | | |
| | 225 | | | | | 230 | | | | | 235 | | | | | | |
| agt | gtg | cag | aga | tgg | gag | gca | agg | agc | ttt | atc | gaa | ata | ttt | gga | caa | 768 | |
| Ser | Val | Gln | Arg | Trp | Glu | Ala | Arg | Ser | Phe | Ile | Glu | Ile | Phe | Gly | Gln | | |
| 240 | | | | | 245 | | | | | 250 | | | | 255 | | | |
| att | gat | tca | gag | ctt | aag | tcg | aat | ttg | agc | aaa | aaa | atg | tta | gag | ttg | 816 | |
| Ile | Asp | Ser | Glu | Leu | Lys | Ser | Asn | Leu | Ser | Lys | Lys | Met | Leu | Glu | Leu | | |
| | | | | 260 | | | | | 265 | | | | | 270 | | | |
| gcg | aaa | ttg | gac | ttc | aat | att | ctg | caa | tgc | aca | cat | cag | aaa | gaa | ctg | 864 | |
| Ala | Lys | Leu | Asp | Phe | Asn | Ile | Leu | Gln | Cys | Thr | His | Gln | Lys | Glu | Leu | | |
| | | | 275 | | | | | 280 | | | | | 285 | | | | |
| cag | att | atc | tca | agg | tgg | ttc | gca | gac | tca | agt | ata | gca | tcc | ctg | aat | 912 | |
| Gln | Ile | Ile | Ser | Arg | Trp | Phe | Ala | Asp | Ser | Ser | Ile | Ala | Ser | Leu | Asn | | |
| | | 290 | | | | | 295 | | | | | 300 | | | | | |
| ttc | tat | cgg | aaa | tgt | tac | gtc | gaa | ttt | tac | ttt | tgg | atg | gct | gca | gcc | 960 | |
| Phe | Tyr | Arg | Lys | Cys | Tyr | Val | Glu | Phe | Tyr | Phe | Trp | Met | Ala | Ala | Ala | | |
| | 305 | | | | | 310 | | | | | 315 | | | | | | |
| atc | tcc | gag | ccg | gag | ttt | tct | gga | agc | aga | gtt | gcc | ttc | aca | aaa | att | 1008 | |
| Ile | Ser | Glu | Pro | Glu | Phe | Ser | Gly | Ser | Arg | Val | Ala | Phe | Thr | Lys | Ile | | |
| 320 | | | | | 325 | | | | | 330 | | | | 335 | | | |
| gct | ata | ctg | atg | aca | atg | cta | gat | gac | ctg | tac | gat | act | cac | gga | acc | 1056 | |
| Ala | Ile | Leu | Met | Thr | Met | Leu | Asp | Asp | Leu | Tyr | Asp | Thr | His | Gly | Thr | | |
| | | | | 340 | | | | | 345 | | | | | 350 | | | |
| ttg | gac | caa | ctc | aaa | atc | ttt | aca | gag | gga | gtg | aga | cga | tgg | gat | gtt | 1104 | |
| Leu | Asp | Gln | Leu | Lys | Ile | Phe | Thr | Glu | Gly | Val | Arg | Arg | Trp | Asp | Val | | |

| 355 | | | | | 360 | | | | | 365 | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|
| tcg | ttg | gta | gag | ggc | ctc | cca | gac | ttc | atg | aaa | att | gca | ttc | gag | ttc | 1152 |
| Ser | Leu | Val | Glu | Gly | Leu | Pro | Asp | Phe | Met | Lys | Ile | Ala | Phe | Glu | Phe | |
| | | 370 | | | | | 375 | | | | | 380 | | | | |
| tgg | tta | aag | aca | tct | aat | gaa | ttg | att | gct | gaa | gct | gtt | aaa | gcg | caa | 1200 |
| Trp | Leu | Lys | Thr | Ser | Asn | Glu | Leu | Ile | Ala | Glu | Ala | Val | Lys | Ala | Gln | |
| | | 385 | | | | 390 | | | | | 395 | | | | | |
| ggg | caa | gat | atg | gcg | gcc | tac | ata | aga | aaa | aat | gca | tgg | gag | cga | tac | 1248 |
| Gly | Gln | Asp | Met | Ala | Ala | Tyr | Ile | Arg | Lys | Asn | Ala | Trp | Glu | Arg | Tyr | |
| 400 | | | | | 405 | | | | | 410 | | | | | 415 | |
| ctt | gaa | gct | tat | ctg | caa | gat | gcg | gaa | tgg | ata | gcc | act | gga | cat | gtc | 1296 |
| Leu | Glu | Ala | Tyr | Leu | Gln | Asp | Ala | Glu | Trp | Ile | Ala | Thr | Gly | His | Val | |
| | | | | 420 | | | | | 425 | | | | | 430 | | |
| ccc | acc | ttt | gat | gag | tac | ttg | aat | aat | ggc | aca | cca | aac | act | ggg | atg | 1344 |
| Pro | Thr | Phe | Asp | Glu | Tyr | Leu | Asn | Asn | Gly | Thr | Pro | Asn | Thr | Gly | Met | |
| | | | 435 | | | | | 440 | | | | | 445 | | | |
| tgt | gta | ttg | aat | ttg | att | ccg | ctt | ctg | tta | atg | ggg | gaa | cat | tta | cca | 1392 |
| Cys | Val | Leu | Asn | Leu | Ile | Pro | Leu | Leu | Leu | Met | Gly | Glu | His | Leu | Pro | |
| | | 450 | | | | | 455 | | | | | 460 | | | | |
| atc | gac | att | ctg | gag | caa | ata | ttc | ttg | ccc | tcc | agg | ttc | cac | cat | ctc | 1440 |
| Ile | Asp | Ile | Leu | Glu | Gln | Ile | Phe | Leu | Pro | Ser | Arg | Phe | His | His | Leu | |
| | 465 | | | | | 470 | | | | | 475 | | | | | |
| att | gaa | ttg | gct | tcc | agg | ctc | gtc | gat | gac | gcg | aga | gat | ttc | cag | gcg | 1488 |
| Ile | Glu | Leu | Ala | Ser | Arg | Leu | Val | Asp | Asp | Ala | Arg | Asp | Phe | Gln | Ala | |
| 480 | | | | | 485 | | | | | 490 | | | | | 495 | |
| gag | aag | gat | cat | ggg | gat | tta | tcg | tgt | att | gag | tgt | tat | tta | aaa | gat | 1536 |
| Glu | Lys | Asp | His | Gly | Asp | Leu | Ser | Cys | Ile | Glu | Cys | Tyr | Leu | Lys | Asp | |
| | | | | 500 | | | | | 505 | | | | | 510 | | |
| cat | cct | gag | tct | aca | gta | gaa | gat | gct | tta | aat | cat | gtt | aat | ggc | ctc | 1584 |
| His | Pro | Glu | Ser | Thr | Val | Glu | Asp | Ala | Leu | Asn | His | Val | Asn | Gly | Leu | |
| | | | 515 | | | | | 520 | | | | | 525 | | | |
| ctt | ggc | aat | tgc | ctt | ctg | gaa | atg | aat | tgg | aag | ttc | tta | aag | aag | cag | 1632 |
| Leu | Gly | Asn | Cys | Leu | Leu | Glu | Met | Asn | Trp | Lys | Phe | Leu | Lys | Lys | Gln | |
| | | 530 | | | | | 535 | | | | | 540 | | | | |
| gac | agt | gtg | cca | ctc | tcg | tgt | aag | aag | tac | agc | ttc | cat | gta | ttg | gca | 1680 |
| Asp | Ser | Val | Pro | Leu | Ser | Cys | Lys | Lys | Tyr | Ser | Phe | His | Val | Leu | Ala | |
| | | 545 | | | | 550 | | | | | 555 | | | | | |
| cga | agc | atc | caa | ttc | atg | tac | aat | caa | ggc | gat | ggc | ttc | tcc | att | tcg | 1728 |
| Arg | Ser | Ile | Gln | Phe | Met | Tyr | Asn | Gln | Gly | Asp | Gly | Phe | Ser | Ile | Ser | |
| 560 | | | | | 565 | | | | | 570 | | | | | 575 | |

aac aaa gtg atc aag gat caa gtg cag aaa gtt ctt att gtc ccc gtg 1776
 Asn Lys Val Ile Lys Asp Gln Val Gln Lys Val Leu Ile Val Pro Val
 580 585 590

cct att tga 1785
 Pro Ile *

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 35 40 45
 Glu Arg Ser Glu Lys Leu Ile Glu Glu Ile Lys Leu Leu Phe Leu Ser
 50 55 60
 Asp Met Asp Asp Ser Cys Asn Asp Ser Asp Arg Asp Leu Ile Lys Arg
 65 70 75 80
 Leu Glu Ile Val Asp Thr Val Glu Cys Leu Gly Ile Asp Arg His Phe
 85 90 95
 Gln Pro Glu Ile Lys Leu Ala Leu Asp Tyr Val Tyr Arg Cys Trp Asn
 100 105 110
 Glu Arg Gly Ile Gly Glu Gly Ser Arg Asp Ser Leu Lys Lys Asp Leu
 115 120 125
 Asn Ala Thr Ala Leu Gly Phe Arg Ala Leu Arg Leu His Arg Tyr Asn
 130 135 140
 Val Ser Ser Gly Val Leu Glu Asn Phe Arg Asp Asp Asn Gly Gln Phe
 145 150 155 160
 Phe Cys Gly Ser Thr Val Glu Glu Glu Gly Ala Glu Ala Tyr Asn Lys
 165 170 175
 His Val Arg Cys Met Leu Ser Leu Ser Arg Ala Ser Asn Ile Leu Phe
 180 185 190
 Pro Gly Glu Lys Val Met Glu Glu Ala Lys Ala Phe Thr Thr Asn Tyr
 195 200 205
 Leu Lys Lys Val Leu Ala Gly Arg Glu Ala Thr His Val Asp Glu Ser
 210 215 220
 Leu Leu Gly Glu Val Lys Tyr Ala Leu Glu Phe Pro Trp His Cys Ser
 225 230 235 240
 Val Gln Arg Trp Glu Ala Arg Ser Phe Ile Glu Ile Phe Gly Gln Ile
 245 250 255
 Asp Ser Glu Leu Lys Ser Asn Leu Ser Lys Lys Met Leu Glu Leu Ala
 260 265 270
 Lys Leu Asp Phe Asn Ile Leu Gln Cys Thr His Gln Lys Glu Leu Gln
 275 280 285
 Ile Ile Ser Arg Trp Phe Ala Asp Ser Ser Ile Ala Ser Leu Asn Phe

```

      290      295      300
Tyr Arg Lys Cys Tyr Val Glu Phe Tyr Phe Trp Met Ala Ala Ala Ile
305      310      315      320
Ser Glu Pro Glu Phe Ser Gly Ser Arg Val Ala Phe Thr Lys Ile Ala
      325      330      335
Ile Leu Met Thr Met Leu Asp Asp Leu Tyr Asp Thr His Gly Thr Leu
      340      345      350
Asp Gln Leu Lys Ile Phe Thr Glu Gly Val Arg Arg Trp Asp Val Ser
      355      360      365
Leu Val Glu Gly Leu Pro Asp Phe Met Lys Ile Ala Phe Glu Phe Trp
      370      375      380
Leu Lys Thr Ser Asn Glu Leu Ile Ala Glu Ala Val Lys Ala Gln Gly
385      390      395      400
Gln Asp Met Ala Ala Tyr Ile Arg Lys Asn Ala Trp Glu Arg Tyr Leu
      405      410      415
Glu Ala Tyr Leu Gln Asp Ala Glu Trp Ile Ala Thr Gly His Val Pro
      420      425      430
Thr Phe Asp Glu Tyr Leu Asn Asn Gly Thr Pro Asn Thr Gly Met Cys
      435      440      445
Val Leu Asn Leu Ile Pro Leu Leu Leu Met Gly Glu His Leu Pro Ile
      450      455      460
Asp Ile Leu Glu Gln Ile Phe Leu Pro Ser Arg Phe His His Leu Ile
465      470      475      480
Glu Leu Ala Ser Arg Leu Val Asp Asp Ala Arg Asp Phe Gln Ala Glu
      485      490      495
Lys Asp His Gly Asp Leu Ser Cys Ile Glu Cys Tyr Leu Lys Asp His
      500      505      510
Pro Glu Ser Thr Val Glu Asp Ala Leu Asn His Val Asn Gly Leu Leu
      515      520      525
Gly Asn Cys Leu Leu Glu Met Asn Trp Lys Phe Leu Lys Lys Gln Asp
      530      535      540
Ser Val Pro Leu Ser Cys Lys Lys Tyr Ser Phe His Val Leu Ala Arg
545      550      555      560
Ser Ile Gln Phe Met Tyr Asn Gln Gly Asp Gly Phe Ser Ile Ser Asn
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Lys Val Ile Lys Asp Gln Val Gln Lys Val Leu Ile Val Pro Val Pro
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Ile

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52

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|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|--|--|--|--|--|--|--|--|--|--|---|--|
| aag | tgt | cgc | ccc | ttg | gct | aat | ttt | cac | cca | tct | gtt | tgg | gga | tat | cat | 100 | | | | | | | | | | | | |
| Lys | Cys | Arg | Pro | Leu | Ala | Asn | Phe | His | Pro | Ser | Val | Trp | Gly | Tyr | His | | | | | | | | | | | | | |
| | | 10 | | | | | 15 | | | | | 20 | | | | | | | | | | | | | | | | |
| ttc | ctt | tct | tat | act | cat | gaa | att | act | aat | caa | gaa | aaa | ggt | gaa | gtt | 148 | | | | | | | | | | | | |
| Phe | Leu | Ser | Tyr | Thr | His | Glu | Ile | Thr | Asn | Gln | Glu | Lys | Val | Glu | Val | | | | | | | | | | | | | |
| | 25 | | | | | 30 | | | | | 35 | | | | | | | | | | | | | | | | | |
| gat | gag | tac | aaa | gag | aca | att | aga | aaa | atg | ctg | gtg | gaa | act | tgc | gac | 196 | | | | | | | | | | | | |
| Asp | Glu | Tyr | Lys | Glu | Thr | Ile | Arg | Lys | Met | Leu | Val | Glu | Thr | Cys | Asp | | | | | | | | | | | | | |
| 40 | | | | | 45 | | | | | 50 | | | | | 55 | | | | | | | | | | | | | |
| aat | agc | act | caa | aag | ctt | gtg | ttg | ata | gac | gcg | atg | caa | cga | ttg | gga | 244 | | | | | | | | | | | | |
| Asn | Ser | Thr | Gln | Lys | Leu | Val | Leu | Ile | Asp | Ala | Met | Gln | Arg | Leu | Gly | | | | | | | | | | | | | |
| | | | | 60 | | | | | 65 | | | | | 70 | | | | | | | | | | | | | | |
| gtg | gct | tat | cat | ttc | gat | aat | gaa | att | gaa | aca | tcc | att | caa | aac | att | 292 | | | | | | | | | | | | |
| Val | Ala | Tyr | His | Phe | Asp | Asn | Glu | Ile | Glu | Thr | Ser | Ile | Gln | Asn | Ile | | | | | | | | | | | | | |
| | | | 75 | | | | 80 | | | | | | 85 | | | | | | | | | | | | | | | |
| ttt | gat | gca | tcg | tcc | aaa | cag | aat | gat | aat | gac | aac | aac | ctt | tac | gtt | 340 | | | | | | | | | | | | |
| Phe | Asp | Ala | Ser | Ser | Lys | Gln | Asn | Asp | Asn | Asp | Asn | Asn | Leu | Tyr | Val | | | | | | | | | | | | | |
| | | 90 | | | | 95 | | | | | | 100 | | | | | | | | | | | | | | | | |
| gtg | tct | ctt | cgt | ttt | cga | ctt | gtg | agg | caa | caa | ggc | cat | tac | atg | tct | 388 | | | | | | | | | | | | |
| Val | Ser | Leu | Arg | Phe | Arg | Leu | Val | Arg | Gln | Gln | Gly | His | Tyr | Met | Ser | | | | | | | | | | | | | |
| | 105 | | | | | 110 | | | | | 115 | | | | | | | | | | | | | | | | | |
| tca | gat | gtg | ttc | aag | caa | ttc | acc | aac | caa | gat | ggg | aaa | ttc | aag | gaa | 436 | | | | | | | | | | | | |
| Ser | Asp | Val | Phe | Lys | Gln | Phe | Thr | Asn | Gln | Asp | Gly | Lys | Phe | Lys | Glu | | | | | | | | | | | | | |
| 120 | | | | | 125 | | | | | 130 | | | | | 135 | | | | | | | | | | | | | |
| aca | ctt | act | aat | gat | gtc | caa | gga | tta | ttg | agt | ttg | tat | gaa | gca | tca | 484 | | | | | | | | | | | | |
| Thr | Leu | Thr | Asn | Asp | Val | Gln | Gly | Leu | Leu | Ser | Leu | Tyr | Glu | Ala | Ser | | | | | | | | | | | | | |
| | | | | 140 | | | | | 145 | | | | | 150 | | | | | | | | | | | | | | |
| cat | ctg | aga | gtg | cgt | aat | gag | gag | att | ctt | gaa | gaa | gct | ctt | aca | ttt | 532 | | | | | | | | | | | | |
| His | Leu | Arg | Val | Arg | Asn | Glu | Glu | Ile | Leu | Glu | Glu | Ala | Leu | Thr | Phe | | | | | | | | | | | | | |
| | | | 155 | | | | | 160 | | | | | 165 | | | | | | | | | | | | | | | |
| acc | acc | act | cat | ctc | gag | tct | att | gtc | tcc | aac | ttg | agc | aat | aat | aat | 580 | | | | | | | | | | | | |
| Thr | Thr | Thr | His | Leu | Glu | Ser | Ile | Val | Ser | Asn | Leu | Ser | Asn | Asn | Asn | | | | | | | | | | | | | |
| | | 170 | | | | | 175 | | | | | 180 | | | | | | | | | | | | | | | | |
| aac | tct | ctt | aag | gtt | gaa | gtt | ggg | gaa | gcc | tta | act | cag | cct | att | cgc | 628 | | | | | | | | | | | | |
| Asn | Ser | Leu | Lys | Val | Glu | Val | Gly | Glu | Ala | Leu | Thr | Gln | Pro | Ile | Arg | | | | | | | | | | | | | |
| | 185 | | | | 190 | | | | | | 195 | | | | | | | | | | | | | | | | | |
| atg | act | tta | cca | agg | atg | gga | gct | aga | aaa | tac | ata | tcc | att | tac | gaa | 676 | | | | | | | | | | | | |
| Met | Thr | Leu | Pro | Arg | Met | Gly | Ala | Arg | Lys | Tyr | Ile | Ser | Ile | Tyr | Glu | | | | | | | | | | | | | |
| 200 | | | | | 205 | | | | | 210 | | | | | 215 | | | | | | | | | | | | | |

| | |
|---|------|
| aac aat gat gca cac cac cat ttg ctt ttg aaa ttt gct aaa ttg gat | 724 |
| Asn Asn Asp Ala His His His Leu Leu Leu Lys Phe Ala Lys Leu Asp | |
| 220 225 230 | |
| ttt aac atg ctg caa aag ttt cac caa aga gag ctt agt gat ctt aca | 772 |
| Phe Asn Met Leu Gln Lys Phe His Gln Arg Glu Leu Ser Asp Leu Thr | |
| 235 240 245 | |
| agg tgg tgg aaa gat ttg gat ttt gca aat aaa tat cca tat gca aga | 820 |
| Arg Trp Trp Lys Asp Leu Asp Phe Ala Asn Lys Tyr Pro Tyr Ala Arg | |
| 250 255 260 | |
| gac agg ttg gtt gag tgt tac ttc tgg ata tta gga gtg tat ttt gag | 868 |
| Asp Arg Leu Val Glu Cys Tyr Phe Trp Ile Leu Gly Val Tyr Phe Glu | |
| 265 270 275 | |
| cca aaa tat agt cgt gcg aga aaa atg atg aca aaa gta ctc aac ctg | 916 |
| Pro Lys Tyr Ser Arg Ala Arg Lys Met Met Thr Lys Val Leu Asn Leu | |
| 280 285 290 295 | |
| acc tcc att att gac gac act ttt gat gct tat gca acc ttt gac gaa | 964 |
| Thr Ser Ile Ile Asp Asp Thr Phe Asp Ala Tyr Ala Thr Phe Asp Glu | |
| 300 305 310 | |
| ctt gtg act ttc aat gat gca atc cag aga tgg gat gct aat gca att | 1012 |
| Leu Val Thr Phe Asn Asp Ala Ile Gln Arg Trp Asp Ala Asn Ala Ile | |
| 315 320 325 | |
| gat tca ata caa cca tat atg aga cct gct tat caa gct ctt cta gac | 1060 |
| Asp Ser Ile Gln Pro Tyr Met Arg Pro Ala Tyr Gln Ala Leu Leu Asp | |
| 330 335 340 | |
| att tac agt gaa atg gaa caa gtg ttg tcc aaa gaa ggt aaa ctg gac | 1108 |
| Ile Tyr Ser Glu Met Glu Gln Val Leu Ser Lys Glu Gly Lys Leu Asp | |
| 345 350 355 | |
| cgt gta tac tat gca aaa aat gag atg aaa aag ttg gtg aga gcc tat | 1156 |
| Arg Val Tyr Tyr Ala Lys Asn Glu Met Lys Lys Leu Val Arg Ala Tyr | |
| 360 365 370 375 | |
| ttt aag gaa acc caa tgg ttg aat gat tgt gac cat att cca aaa tat | 1204 |
| Phe Lys Glu Thr Gln Trp Leu Asn Asp Cys Asp His Ile Pro Lys Tyr | |
| 380 385 390 | |
| gag gaa caa gtg gag aat gca atc gta agt gct ggc tat atg atg ata | 1252 |
| Glu Glu Gln Val Glu Asn Ala Ile Val Ser Ala Gly Tyr Met Met Ile | |
| 395 400 405 | |
| tca aca act tgc ttg gtc ggt ata gaa gaa ttt ata tcc cac gag act | 1300 |
| Ser Thr Thr Cys Leu Val Gly Ile Glu Glu Phe Ile Ser His Glu Thr | |
| 410 415 420 | |

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ttt gaa tgg ttg atg aat gag tct gtg att gtt cga gct tcc gca ttg      1348
Phe Glu Trp Leu Met Asn Glu Ser Val Ile Val Arg Ala Ser Ala Leu
    425                      430                      435

att gcc aga gca atg aac gat att gtt gga cat gaa gat gaa caa gaa      1396
Ile Ala Arg Ala Met Asn Asp Ile Val Gly His Glu Asp Glu Gln Glu
    440                      445                      450                      455

aga gga cat gta gct tca ctt att gaa tgt tac atg aaa gat tat gga      1444
Arg Gly His Val Ala Ser Leu Ile Glu Cys Tyr Met Lys Asp Tyr Gly
                      460                      465                      470

gct tca aag caa gag act tac att aag ttc ctg aaa gag gtc acc aat      1492
Ala Ser Lys Gln Glu Thr Tyr Ile Lys Phe Leu Lys Glu Val Thr Asn
                      475                      480                      485

gca tgg aag gac ata aac aaa caa ttc tcc cgt cca act gaa gta cca      1540
Ala Trp Lys Asp Ile Asn Lys Gln Phe Ser Arg Pro Thr Glu Val Pro
    490                      495                      500

atg ttt gtc ctt gaa cga gtt cta aat ttg aca cgt gtg gct gac acg      1588
Met Phe Val Leu Glu Arg Val Leu Asn Leu Thr Arg Val Ala Asp Thr
    505                      510                      515

tta tat aag gag aaa gat aca tat tca acc gcc aaa gga aaa ctt aaa      1636
Leu Tyr Lys Glu Lys Asp Thr Tyr Ser Thr Ala Lys Gly Lys Leu Lys
    520                      525                      530                      535

aac atg att aat cca ata cta att gaa tct gtc aaa ata taa      1678
Asn Met Ile Asn Pro Ile Leu Ile Glu Ser Val Lys Ile *
                      540                      545

atataatgct gaaattgcac cttcatcatc caactatttca cagcaaaaata aggcataata 1738
taaattgaag actcacaaca tatgagttgt taattcctgg gatgtttgaa ataaacaata 1798
attgttttta ttttaatttgc taagccaaag tgaaatatac aacacttgag ttgtattaaa 1858
tcatgtttta tctcatttcc agcttgtgag tttggattat tatattgtta attatcatca 1918
ctttataatg tactgtaatc gtattgtatt tgtattgtag tgttgtcata ataaaatttg 1978
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<211> 548

<212> PRT

<213> Lycopersicon esculentum

<400> 52

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Pro Ser Val Trp Gly Tyr His Phe Leu Ser Tyr Thr His Glu Ile Thr
    20          25          30
Asn Gln Glu Lys Val Glu Val Asp Glu Tyr Lys Glu Thr Ile Arg Lys
    35          40          45
Met Leu Val Glu Thr Cys Asp Asn Ser Thr Gln Lys Leu Val Leu Ile
    50          55          60

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| | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| Asp | Ala | Met | Gln | Arg | Leu | Gly | Val | Ala | Tyr | His | Phe | Asp | Asn | Glu | Ile |
| 65 | | | | | 70 | | | | | 75 | | | | | 80 |
| Glu | Thr | Ser | Ile | Gln | Asn | Ile | Phe | Asp | Ala | Ser | Ser | Lys | Gln | Asn | Asp |
| | | | | 85 | | | | 90 | | | | | | 95 | |
| Asn | Asp | Asn | Asn | Leu | Tyr | Val | Val | Ser | Leu | Arg | Phe | Arg | Leu | Val | Arg |
| | | | 100 | | | | | 105 | | | | | 110 | | |
| Gln | Gln | Gly | His | Tyr | Met | Ser | Ser | Asp | Val | Phe | Lys | Gln | Phe | Thr | Asn |
| | | 115 | | | | | 120 | | | | | 125 | | | |
| Gln | Asp | Gly | Lys | Phe | Lys | Glu | Thr | Leu | Thr | Asn | Asp | Val | Gln | Gly | Leu |
| | 130 | | | | | 135 | | | | | 140 | | | | |
| Leu | Ser | Leu | Tyr | Glu | Ala | Ser | His | Leu | Arg | Val | Arg | Asn | Glu | Glu | Ile |
| 145 | | | | 150 | | | | | | 155 | | | | | 160 |
| Leu | Glu | Glu | Ala | Leu | Thr | Phe | Thr | Thr | Thr | His | Leu | Glu | Ser | Ile | Val |
| | | | | 165 | | | | | 170 | | | | | 175 | |
| Ser | Asn | Leu | Ser | Asn | Asn | Asn | Asn | Ser | Leu | Lys | Val | Glu | Val | Gly | Glu |
| | | | 180 | | | | | 185 | | | | | 190 | | |
| Ala | Leu | Thr | Gln | Pro | Ile | Arg | Met | Thr | Leu | Pro | Arg | Met | Gly | Ala | Arg |
| | | 195 | | | | | 200 | | | | | 205 | | | |
| Lys | Tyr | Ile | Ser | Ile | Tyr | Glu | Asn | Asn | Asp | Ala | His | His | His | Leu | Leu |
| | 210 | | | | | 215 | | | | | 220 | | | | |
| Leu | Lys | Phe | Ala | Lys | Leu | Asp | Phe | Asn | Met | Leu | Gln | Lys | Phe | His | Gln |
| 225 | | | | 230 | | | | | | 235 | | | | | 240 |
| Arg | Glu | Leu | Ser | Asp | Leu | Thr | Arg | Trp | Trp | Lys | Asp | Leu | Asp | Phe | Ala |
| | | | | 245 | | | | 250 | | | | | | 255 | |
| Asn | Lys | Tyr | Pro | Tyr | Ala | Arg | Asp | Arg | Leu | Val | Glu | Cys | Tyr | Phe | Trp |
| | | | 260 | | | | 265 | | | | | | 270 | | |
| Ile | Leu | Gly | Val | Tyr | Phe | Glu | Pro | Lys | Tyr | Ser | Arg | Ala | Arg | Lys | Met |
| | | 275 | | | | | 280 | | | | | 285 | | | |
| Met | Thr | Lys | Val | Leu | Asn | Leu | Thr | Ser | Ile | Ile | Asp | Asp | Thr | Phe | Asp |
| | 290 | | | | | 295 | | | | | 300 | | | | |
| Ala | Tyr | Ala | Thr | Phe | Asp | Glu | Leu | Val | Thr | Phe | Asn | Asp | Ala | Ile | Gln |
| 305 | | | | | 310 | | | | | 315 | | | | | 320 |
| Arg | Trp | Asp | Ala | Asn | Ala | Ile | Asp | Ser | Ile | Gln | Pro | Tyr | Met | Arg | Pro |
| | | | | 325 | | | | | 330 | | | | | 335 | |
| Ala | Tyr | Gln | Ala | Leu | Leu | Asp | Ile | Tyr | Ser | Glu | Met | Glu | Gln | Val | Leu |
| | | | 340 | | | | | 345 | | | | | 350 | | |
| Ser | Lys | Glu | Gly | Lys | Leu | Asp | Arg | Val | Tyr | Tyr | Ala | Lys | Asn | Glu | Met |
| | | 355 | | | | | 360 | | | | | 365 | | | |
| Lys | Lys | Leu | Val | Arg | Ala | Tyr | Phe | Lys | Glu | Thr | Gln | Trp | Leu | Asn | Asp |
| | 370 | | | | | 375 | | | | | 380 | | | | |
| Cys | Asp | His | Ile | Pro | Lys | Tyr | Glu | Glu | Gln | Val | Glu | Asn | Ala | Ile | Val |
| 385 | | | | | 390 | | | | | 395 | | | | | 400 |
| Ser | Ala | Gly | Tyr | Met | Met | Ile | Ser | Thr | Thr | Cys | Leu | Val | Gly | Ile | Glu |
| | | | | 405 | | | | | 410 | | | | | 415 | |
| Glu | Phe | Ile | Ser | His | Glu | Thr | Phe | Glu | Trp | Leu | Met | Asn | Glu | Ser | Val |
| | | | 420 | | | | | 425 | | | | | 430 | | |
| Ile | Val | Arg | Ala | Ser | Ala | Leu | Ile | Ala | Arg | Ala | Met | Asn | Asp | Ile | Val |
| | | 435 | | | | | 440 | | | | | 445 | | | |
| Gly | His | Glu | Asp | Glu | Gln | Glu | Arg | Gly | His | Val | Ala | Ser | Leu | Ile | Glu |
| | 450 | | | | | 455 | | | | | 460 | | | | |
| Cys | Tyr | Met | Lys | Asp | Tyr | Gly | Ala | Ser | Lys | Gln | Glu | Thr | Tyr | Ile | Lys |
| 465 | | | | | 470 | | | | | 475 | | | | | 480 |
| Phe | Leu | Lys | Glu | Val | Thr | Asn | Ala | Trp | Lys | Asp | Ile | Asn | Lys | Gln | Phe |

| | | | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| Ser | Arg | Pro | Thr | 485 | Glu | Val | Pro | Met | Phe | 490 | Val | Leu | Glu | Arg | Val | 495 | Leu | Asn |
| | | | 500 | | | | | | 505 | | | | | | | 510 | | |
| Leu | Thr | Arg | Val | Ala | Asp | Thr | Leu | Tyr | Lys | Glu | Lys | Asp | Thr | Tyr | Ser | | | |
| | | 515 | | | | | 520 | | | | | 525 | | | | | | |
| Thr | Ala | Lys | Gly | Lys | Leu | Lys | Asn | Met | Ile | Asn | Pro | Ile | Leu | Ile | Glu | | | |
| | | 530 | | | | 535 | | | | | 540 | | | | | | | |
| Ser | Val | Lys | Ile | | | | | | | | | | | | | | | |
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<210> 53
 <211> 1912
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 <213> *Salvia officinalis*

 <220>
 <221> CDS
 <222> (26)...(1798)
 <223> (+)-sabinene syntase

| | | | | | | | | | | | | | | | | | |
|------------|--------|------|-------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|--|-----|
| <400> 53 | | | | | | | | | | | | | | | | | |
| agcaatatta | caacta | acaa | taaaa | atg | tct | tcc | att | agc | ata | aac | ata | gct | | | | | 52 |
| | | | | Met | Ser | Ser | Ile | Ser | Ile | Asn | Ile | Ala | | | | | |
| | | | | 1 | | | | 5 | | | | | | | | | |
| atg | cca | ctg | aat | tcc | ctc | cac | aac | ttt | gag | agg | aaa | cct | tca | aaa | gca | | 100 |
| Met | Pro | Leu | Asn | Ser | Leu | His | Asn | Phe | Glu | Arg | Lys | Pro | Ser | Lys | Ala | | |
| 10 | | | | 15 | | | | 20 | | | | | | | 25 | | |
| tgg | tct | acc | tct | tgc | act | gca | ccc | gca | gct | cgc | ctc | cgg | gca | tct | tcc | | 148 |
| Trp | Ser | Thr | Ser | Cys | Thr | Ala | Pro | Ala | Ala | Arg | Leu | Arg | Ala | Ser | Ser | | |
| | | | | 30 | | | | 35 | | | | | | 40 | | | |
| tcc | tta | caa | caa | gaa | aaa | cct | cac | caa | atc | cga | cgc | tct | ggg | gat | tac | | 196 |
| Ser | Leu | Gln | Gln | Glu | Lys | Pro | His | Gln | Ile | Arg | Arg | Ser | Gly | Asp | Tyr | | |
| | | | 45 | | | | | 50 | | | | | 55 | | | | |
| caa | ccc | tct | ctt | tgg | gat | ttc | aat | tac | ata | cag | tct | ctc | aac | act | ccg | | 244 |
| Gln | Pro | Ser | Leu | Trp | Asp | Phe | Asn | Tyr | Ile | Gln | Ser | Leu | Asn | Thr | Pro | | |
| | | 60 | | | | 65 | | | | | | 70 | | | | | |
| tat | aag | gag | cag | aga | cac | ttt | aat | agg | caa | gca | gag | ttg | att | atg | caa | | 292 |
| Tyr | Lys | Glu | Gln | Arg | His | Phe | Asn | Arg | Gln | Ala | Glu | Leu | Ile | Met | Gln | | |
| | 75 | | | | 80 | | | | | | 85 | | | | | | |
| gtg | agg | atg | ttg | ctc | aag | gta | aag | atg | gag | gca | att | caa | cag | ttg | gag | | 340 |
| Val | Arg | Met | Leu | Leu | Lys | Val | Lys | Met | Glu | Ala | Ile | Gln | Gln | Leu | Glu | | |
| 90 | | | | 95 | | | | | 100 | | | | | 105 | | | |
| ttg | att | gat | gac | ttg | caa | tac | ctg | gga | ctg | tct | tat | ttc | ttt | caa | gat | | 388 |
| Leu | Ile | Asp | Asp | Leu | Gln | Tyr | Leu | Gly | Leu | Ser | Tyr | Phe | Phe | Gln | Asp | | |
| | | | | 110 | | | | | 115 | | | | | 120 | | | |

| | |
|---|------|
| gag att aaa caa atc tta agt tct ata cac aat gag ccc aga tat ttc | 436 |
| Glu Ile Lys Gln Ile Leu Ser Ser Ile His Asn Glu Pro Arg Tyr Phe | |
| 125 130 135 | |
| cac aat aat gat ttg tat ttc aca gct ctt gga ttc aga atc ctc aga | 484 |
| His Asn Asn Asp Leu Tyr Phe Thr Ala Leu Gly Phe Arg Ile Leu Arg | |
| 140 145 150 | |
| caa cat ggt ttt aat gtt tcc gaa gat gta ttt gat tgt ttc aaa att | 532 |
| Gln His Gly Phe Asn Val Ser Glu Asp Val Phe Asp Cys Phe Lys Ile | |
| 155 160 165 | |
| gag aag tgc agt gat ttc aat gca aac ctt gct caa gat acg aag gga | 580 |
| Glu Lys Cys Ser Asp Phe Asn Ala Asn Leu Ala Gln Asp Thr Lys Gly | |
| 170 175 180 185 | |
| atg tta caa ctt tat gaa gca tct ttc ctt ttg aga gaa ggt gaa gat | 628 |
| Met Leu Gln Leu Tyr Glu Ala Ser Phe Leu Leu Arg Glu Gly Glu Asp | |
| 190 195 200 | |
| aca ttg gag cta gca aga cga ttt tcc acc aga tct cta cga gaa aaa | 676 |
| Thr Leu Glu Leu Ala Arg Arg Phe Ser Thr Arg Ser Leu Arg Glu Lys | |
| 205 210 215 | |
| ttt gat gaa ggt ggt gat gaa att gat gaa gat cta tca tcg tgg att | 724 |
| Phe Asp Glu Gly Gly Asp Glu Ile Asp Glu Asp Leu Ser Ser Trp Ile | |
| 220 225 230 | |
| cgc cat tcc ttg gat ctt cct ctt cat tgg agg gtc caa gga tta gag | 772 |
| Arg His Ser Leu Asp Leu Pro Leu His Trp Arg Val Gln Gly Leu Glu | |
| 235 240 245 | |
| gca aga tgg ttc tta gat gct tat gcg agg agg ccg gac atg aat cca | 820 |
| Ala Arg Trp Phe Leu Asp Ala Tyr Ala Arg Arg Pro Asp Met Asn Pro | |
| 250 255 260 265 | |
| ctt att ttc aaa ctc gcc aaa ctc aac ttc aat att gtt cag gca aca | 868 |
| Leu Ile Phe Lys Leu Ala Lys Leu Asn Phe Asn Ile Val Gln Ala Thr | |
| 270 275 280 | |
| tat caa gaa gaa ctg aaa gat atc tca agg tgg tgg aat agt tcg tgc | 916 |
| Tyr Gln Glu Glu Leu Lys Asp Ile Ser Arg Trp Trp Asn Ser Ser Cys | |
| 285 290 295 | |
| ctt gct gag aaa ctc cca ttt gtg aga gat agg att gtg gaa tgc ttc | 964 |
| Leu Ala Glu Lys Leu Pro Phe Val Arg Asp Arg Ile Val Glu Cys Phe | |
| 300 305 310 | |
| ttt tgg gcc atc gcg gct ttt gag cct cac caa tat agt tat cag aga | 1012 |
| Phe Trp Ala Ile Ala Ala Phe Glu Pro His Gln Tyr Ser Tyr Gln Arg | |
| 315 320 325 | |
| aaa atg gcc gcc gtt att att act ttc ata aca att atc gat gat gtt | 1060 |

| | | | | | | | | | | | | | | | | |
|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|-----|------------|------------|------------|------|
| Lys 330 | Met | Ala | Ala | Val | Ile 335 | Ile | Thr | Phe | Ile | Thr 340 | Ile | Ile | Asp | Asp | Val 345 | |
| tat | gat | gtg | tat | gga | aca | ata | gaa | gaa | cta | gaa | cta | tta | aca | gat | atg | 1108 |
| Tyr | Asp | Val | Tyr | Gly 350 | Thr | Ile | Glu | Glu | Leu 355 | Glu | Leu | Leu | Thr | Asp 360 | Met | |
| att | cgc | aga | tgg | gat | aat | aaa | tca | ata | agc | caa | ctt | cca | tat | tat | atg | 1156 |
| Ile | Arg | Arg | Trp 365 | Asp | Asn | Lys | Ser | Ile | Ser | Gln | Leu | Pro | Tyr 375 | Tyr | Met | |
| caa | gtg | tgc | tat | ttg | gca | cta | tac | aac | ttc | gtt | tct | gag | cgg | gct | tac | 1204 |
| Gln | Val | Cys 380 | Tyr | Leu | Ala | Leu | Tyr 385 | Asn | Phe | Val | Ser | Glu | Arg | Ala | Tyr | |
| gat | att | cta | aaa | gat | caa | cat | ttc | aac | agc | atc | cca | tat | tta | cag | aga | 1252 |
| Asp | Ile 395 | Leu | Lys | Asp | Gln | His 400 | Phe | Asn | Ser | Ile | Pro 405 | Tyr | Leu | Gln | Arg | |
| tcg | tgg | gta | agt | ttg | gtt | gaa | gga | tat | ctt | aag | gag | gca | tac | tgg | tac | 1300 |
| Ser | Trp | Val | Ser | Leu | Val 415 | Glu | Gly | Tyr | Leu | Lys 420 | Glu | Ala | Tyr | Trp | Tyr 425 | |
| tac | aat | ggc | tat | aaa | cca | agc | ttg | gaa | gaa | tat | ctc | aac | aac | gcc | aag | 1348 |
| Tyr | Asn | Gly | Tyr | Lys 430 | Pro | Ser | Leu | Glu | Glu 435 | Tyr | Leu | Asn | Asn | Ala 440 | Lys | |
| att | tca | ata | tcg | gct | cct | aca | atc | ata | tcc | cag | ctt | tat | ttt | aca | tta | 1396 |
| Ile | Ser | Ile | Ser 445 | Ala | Pro | Thr | Ile | Ile | Ser | Gln | Leu | Tyr | Phe 455 | Thr | Leu | |
| gca | aac | tcg | att | gat | gaa | aca | gct | atc | gag | agc | ttg | tac | caa | tat | cat | 1444 |
| Ala | Asn | Ser 460 | Ile | Asp | Glu | Thr | Ala 465 | Ile | Glu | Ser | Leu | Tyr | Gln | Tyr | His | |
| aac | ata | ctt | tac | cta | tca | gga | acc | ata | tta | agg | ctt | gct | gac | gat | ctt | 1492 |
| Asn | Ile 475 | Leu | Tyr | Leu | Ser | Gly 480 | Thr | Ile | Leu | Arg | Leu 485 | Ala | Asp | Asp | Leu | |
| ggg | aca | tca | caa | cat | gag | ctg | gag | aga | gga | gac | gta | ccg | aaa | gca | atc | 1540 |
| Gly | Thr | Ser | Gln | His | Glu | Leu | Glu | Arg | Gly | Asp 500 | Val | Pro | Lys | Ala | Ile 505 | |
| cag | tgc | tac | atg | aat | gac | aca | aat | gct | tcg | gag | aga | gag | gcg | gtg | gaa | 1588 |
| Gln | Cys | Tyr | Met | Asn 510 | Asp | Thr | Asn | Ala | Ser 515 | Glu | Arg | Glu | Ala | Val 520 | Glu | |
| cac | gtg | aag | ttt | ctg | ata | agg | gag | gcg | tgg | aag | gag | atg | aac | acg | gtc | 1636 |
| His | Val | Lys 525 | Phe | Leu | Ile | Arg | Glu | Ala 530 | Trp | Lys | Glu | Met | Asn 535 | Thr | Val | |
| aca | aca | gcc | agc | gat | tgt | ccg | ttt | acg | gat | gat | ttg | gtt | gcg | gcc | gca | 1684 |
| Thr | Thr | Ala | Ser | Asp | Cys | Pro | Phe | Thr | Asp | Asp | Leu | Val | Ala | Ala | Ala | |

| | | | |
|--|-----|-----|------|
| 540 | 545 | 550 | |
| gct aat ctt gca agg gcg gct cag ttt ata tat ctc gac ggg gat ggg | | | 1732 |
| Ala Asn Leu Ala Arg Ala Ala Gln Phe Ile Tyr Leu Asp Gly Asp Gly | | | |
| 555 | 560 | 565 | |
| cat ggc gtg caa cac tca gaa ata cat caa cag atg gga ggc ctg cta | | | 1780 |
| His Gly Val Gln His Ser Glu Ile His Gln Gln Met Gly Gly Leu Leu | | | |
| 570 | 575 | 580 | 585 |
| ttc cag cct tat gtc tga ataaatcgaa aatccaacct actatgtatc | | | 1828 |
| Phe Gln Pro Tyr Val * | | | |
| 590 | | | |
| cctcgataat atattcttgg ggtaacatg tttaattaaa gttctaattd aaagagctga | | | 1888 |
| atcgatcctc aaaaaaaaaa aaaa | | | 1912 |

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 <212> PRT
 <213> Salvia officinalis

<400> 54

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| Asn Phe Glu Arg Lys Pro Ser Lys Ala Trp Ser Thr Ser Cys Thr Ala | |
| 20 25 30 | |
| Pro Ala Ala Arg Leu Arg Ala Ser Ser Ser Leu Gln Gln Glu Lys Pro | |
| 35 40 45 | |
| His Gln Ile Arg Arg Ser Gly Asp Tyr Gln Pro Ser Leu Trp Asp Phe | |
| 50 55 60 | |
| Asn Tyr Ile Gln Ser Leu Asn Thr Pro Tyr Lys Glu Gln Arg His Phe | |
| 65 70 75 80 | |
| Asn Arg Gln Ala Glu Leu Ile Met Gln Val Arg Met Leu Leu Lys Val | |
| 85 90 95 | |
| Lys Met Glu Ala Ile Gln Gln Leu Glu Leu Ile Asp Asp Leu Gln Tyr | |
| 100 105 110 | |
| Leu Gly Leu Ser Tyr Phe Phe Gln Asp Glu Ile Lys Gln Ile Leu Ser | |
| 115 120 125 | |
| Ser Ile His Asn Glu Pro Arg Tyr Phe His Asn Asn Asp Leu Tyr Phe | |
| 130 135 140 | |
| Thr Ala Leu Gly Phe Arg Ile Leu Arg Gln His Gly Phe Asn Val Ser | |
| 145 150 155 160 | |
| Glu Asp Val Phe Asp Cys Phe Lys Ile Glu Lys Cys Ser Asp Phe Asn | |
| 165 170 175 | |
| Ala Asn Leu Ala Gln Asp Thr Lys Gly Met Leu Gln Leu Tyr Glu Ala | |
| 180 185 190 | |
| Ser Phe Leu Leu Arg Glu Gly Glu Asp Thr Leu Glu Leu Ala Arg Arg | |
| 195 200 205 | |
| Phe Ser Thr Arg Ser Leu Arg Glu Lys Phe Asp Glu Gly Gly Asp Glu | |
| 210 215 220 | |
| Ile Asp Glu Asp Leu Ser Ser Trp Ile Arg His Ser Leu Asp Leu Pro | |
| 225 230 235 240 | |

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Leu His Trp Arg Val Gln Gly Leu Glu Ala Arg Trp Phe Leu Asp Ala
                245                250
Tyr Ala Arg Arg Pro Asp Met Asn Pro Leu Ile Phe Lys Leu Ala Lys
                260                265
Leu Asn Phe Asn Ile Val Gln Ala Thr Tyr Gln Glu Glu Leu Lys Asp
                275                280                285
Ile Ser Arg Trp Trp Asn Ser Ser Cys Leu Ala Glu Lys Leu Pro Phe
                290                295                300
Val Arg Asp Arg Ile Val Glu Cys Phe Phe Trp Ala Ile Ala Ala Phe
305                310                315                320
Glu Pro His Gln Tyr Ser Tyr Gln Arg Lys Met Ala Ala Val Ile Ile
                325                330                335
Thr Phe Ile Thr Ile Ile Asp Asp Val Tyr Asp Val Tyr Gly Thr Ile
                340                345                350
Glu Glu Leu Glu Leu Leu Thr Asp Met Ile Arg Arg Trp Asp Asn Lys
                355                360                365
Ser Ile Ser Gln Leu Pro Tyr Tyr Met Gln Val Cys Tyr Leu Ala Leu
370                375                380
Tyr Asn Phe Val Ser Glu Arg Ala Tyr Asp Ile Leu Lys Asp Gln His
385                390                395                400
Phe Asn Ser Ile Pro Tyr Leu Gln Arg Ser Trp Val Ser Leu Val Glu
                405                410                415
Gly Tyr Leu Lys Glu Ala Tyr Trp Tyr Tyr Asn Gly Tyr Lys Pro Ser
                420                425                430
Leu Glu Glu Tyr Leu Asn Asn Ala Lys Ile Ser Ile Ser Ala Pro Thr
                435                440                445
Ile Ile Ser Gln Leu Tyr Phe Thr Leu Ala Asn Ser Ile Asp Glu Thr
450                455                460
Ala Ile Glu Ser Leu Tyr Gln Tyr His Asn Ile Leu Tyr Leu Ser Gly
465                470                475                480
Thr Ile Leu Arg Leu Ala Asp Asp Leu Gly Thr Ser Gln His Glu Leu
                485                490                495
Glu Arg Gly Asp Val Pro Lys Ala Ile Gln Cys Tyr Met Asn Asp Thr
                500                505                510
Asn Ala Ser Glu Arg Glu Ala Val Glu His Val Lys Phe Leu Ile Arg
                515                520                525
Glu Ala Trp Lys Glu Met Asn Thr Val Thr Thr Ala Ser Asp Cys Pro
530                535                540
Phe Thr Asp Asp Leu Val Ala Ala Ala Asn Leu Ala Arg Ala Ala
545                550                555                560
Gln Phe Ile Tyr Leu Asp Gly Asp Gly His Gly Val Gln His Ser Glu
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Ile His Gln Gln Met Gly Gly Leu Leu Phe Gln Pro Tyr Val
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<213> Abies grandis

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<221> CDS
<222> (3)...(2609)

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<223> abietadiene synthase

<400> 55

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| Met Ala Met Pro Ser Ser Ser Leu Ser Ser Gln Ile Pro Thr Ala | |
| 1 5 10 15 | |
| gct cat cat cta act gct aac gca caa tcc att ccg cat ttc tcc acg | 95 |
| Ala His His Leu Thr Ala Asn Ala Gln Ser Ile Pro His Phe Ser Thr | |
| 20 25 30 | |
| acg ctg aat gct gga agc agt gct agc aaa cgg aga agc ttg tac cta | 143 |
| Thr Leu Asn Ala Gly Ser Ser Ala Ser Lys Arg Arg Ser Leu Tyr Leu | |
| 35 40 45 | |
| cga tgg ggt aaa ggt tca aac aag atc att gcc tgt gtt gga gaa ggt | 191 |
| Arg Trp Gly Lys Gly Ser Asn Lys Ile Ile Ala Cys Val Gly Glu Gly | |
| 50 55 60 | |
| ggt gca acc tct gtt cct tat cag tct gct gaa aag aat gat tcg ctt | 239 |
| Gly Ala Thr Ser Val Pro Tyr Gln Ser Ala Glu Lys Asn Asp Ser Leu | |
| 65 70 75 | |
| tct tct tct aca ttg gtg aaa cga gaa ttt cct cca gga ttt tgg aag | 287 |
| Ser Ser Ser Thr Leu Val Lys Arg Glu Phe Pro Pro Gly Phe Trp Lys | |
| 80 85 90 95 | |
| gat gat ctt atc gat tct cta acg tca tct cac aag gtt gca gca tca | 335 |
| Asp Asp Leu Ile Asp Ser Leu Thr Ser Ser His Lys Val Ala Ala Ser | |
| 100 105 110 | |
| gac gag aag cgt atc gag aca tta ata tcc gag att aag aat atg ttt | 383 |
| Asp Glu Lys Arg Ile Glu Thr Leu Ile Ser Glu Ile Lys Asn Met Phe | |
| 115 120 125 | |
| aga tgt atg ggc tat ggc gaa acg aat ccc tct gca tat gac act gct | 431 |
| Arg Cys Met Gly Tyr Gly Glu Thr Asn Pro Ser Ala Tyr Asp Thr Ala | |
| 130 135 140 | |
| tgg gta gca agg att cca gca gtt gat ggc tct gac aac cct cac ttt | 479 |
| Trp Val Ala Arg Ile Pro Ala Val Asp Gly Ser Asp Asn Pro His Phe | |
| 145 150 155 | |
| cct gag acg gtt gaa tgg att ctt caa aat cag ttg aaa gat ggg tct | 527 |
| Pro Glu Thr Val Glu Trp Ile Leu Gln Asn Gln Leu Lys Asp Gly Ser | |
| 160 165 170 175 | |
| tgg ggt gaa gga ttc tac ttc ttg gca tat gac aga ata ctg gct aca | 575 |
| Trp Gly Glu Gly Phe Tyr Phe Leu Ala Tyr Asp Arg Ile Leu Ala Thr | |
| 180 185 190 | |
| ctt gca tgt att att acc ctt acc ctc tgg cgt act ggg gag aca caa | 623 |
| Leu Ala Cys Ile Ile Thr Leu Thr Leu Trp Arg Thr Gly Glu Thr Gln | |

| 195 | | | | | | | | | | 200 | | | | | 205 | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|--|--|--|--|
| gta | cag | aaa | ggt | att | gaa | ttc | ttc | agg | aca | caa | gct | gga | aag | atg | gaa | 671 | | | | |
| Val | Gln | Lys | Gly | Ile | Glu | Phe | Phe | Arg | Thr | Gln | Ala | Gly | Lys | Met | Glu | | | | | |
| | | 210 | | | | | 215 | | | | | 220 | | | | | | | | |
| gat | gaa | gct | gat | agt | cat | agg | cca | agt | gga | ttt | gaa | ata | gta | ttt | cct | 719 | | | | |
| Asp | Glu | Ala | Asp | Ser | His | Arg | Pro | Ser | Gly | Phe | Glu | Ile | Val | Phe | Pro | | | | | |
| | 225 | | | | | 230 | | | | | 235 | | | | | | | | | |
| gca | atg | cta | aag | gaa | gct | aaa | atc | tta | ggc | ttg | gat | ctg | cct | tac | gat | 767 | | | | |
| Ala | Met | Leu | Lys | Glu | Ala | Lys | Ile | Leu | Gly | Leu | Asp | Leu | Pro | Tyr | Asp | | | | | |
| 240 | | | | | 245 | | | | | 250 | | | | | 255 | | | | | |
| ttg | cca | ttc | ctg | aaa | caa | atc | atc | gaa | aag | cgg | gag | gct | aag | ctt | aaa | 815 | | | | |
| Leu | Pro | Phe | Leu | Lys | Gln | Ile | Ile | Glu | Lys | Arg | Glu | Ala | Lys | Leu | Lys | | | | | |
| | | | | 260 | | | | | 265 | | | | | 270 | | | | | | |
| agg | att | ccc | act | gat | gtt | ctc | tat | gcc | ctt | cca | aca | acg | tta | ttg | tat | 863 | | | | |
| Arg | Ile | Pro | Thr | Asp | Val | Leu | Tyr | Ala | Leu | Pro | Thr | Thr | Leu | Leu | Tyr | | | | | |
| | | | 275 | | | | | 280 | | | | | 285 | | | | | | | |
| tct | ttg | gaa | ggt | tta | caa | gaa | ata | gta | gac | tgg | cag | aaa | ata | atg | aaa | 911 | | | | |
| Ser | Leu | Glu | Gly | Leu | Gln | Glu | Ile | Val | Asp | Trp | Gln | Lys | Ile | Met | Lys | | | | | |
| | 290 | | | | | | 295 | | | | | 300 | | | | | | | | |
| ctt | caa | tcc | aag | gat | gga | tca | ttt | ctc | agc | tct | ccg | gca | tct | aca | gcg | 959 | | | | |
| Leu | Gln | Ser | Lys | Asp | Gly | Ser | Phe | Leu | Ser | Ser | Pro | Ala | Ser | Thr | Ala | | | | | |
| | 305 | | | | | 310 | | | | | 315 | | | | | | | | | |
| gct | gta | ttc | atg | cgt | aca | ggg | aac | aaa | aag | tgc | ttg | gat | ttc | ttg | aac | 1007 | | | | |
| Ala | Val | Phe | Met | Arg | Thr | Gly | Asn | Lys | Lys | Cys | Leu | Asp | Phe | Leu | Asn | | | | | |
| 320 | | | | | 325 | | | | | 330 | | | | | 335 | | | | | |
| ttt | gtc | ttg | aag | aaa | ttc | gga | aac | cat | gtg | cct | tgt | cac | tat | ccg | ctt | 1055 | | | | |
| Phe | Val | Leu | Lys | Lys | Phe | Gly | Asn | His | Val | Pro | Cys | His | Tyr | Pro | Leu | | | | | |
| | | | | 340 | | | | | 345 | | | | | 350 | | | | | | |
| gat | cta | ttt | gaa | cgt | ttg | tgg | gcg | gtt | gat | aca | gtt | gag | cgg | cta | ggt | 1103 | | | | |
| Asp | Leu | Phe | Glu | Arg | Leu | Trp | Ala | Val | Asp | Thr | Val | Glu | Arg | Leu | Gly | | | | | |
| | | | 355 | | | | | 360 | | | | | 365 | | | | | | | |
| atc | gat | cgt | cat | ttc | aaa | gag | gag | atc | aag | gaa | gca | ttg | gat | tat | gtt | 1151 | | | | |
| Ile | Asp | Arg | His | Phe | Lys | Glu | Glu | Ile | Lys | Glu | Ala | Leu | Asp | Tyr | Val | | | | | |
| | | 370 | | | | | 375 | | | | | 380 | | | | | | | | |
| tac | agc | cat | tgg | gac | gaa | aga | ggc | att | gga | tgg | gcg | aga | gag | aat | cct | 1199 | | | | |
| Tyr | Ser | His | Trp | Asp | Glu | Arg | Gly | Ile | Gly | Trp | Ala | Arg | Glu | Asn | Pro | | | | | |
| | 385 | | | | | 390 | | | | | 395 | | | | | | | | | |
| gtt | cct | gat | att | gat | gat | aca | gcc | atg | ggc | ctt | cga | atc | ttg | aga | tta | 1247 | | | | |
| Val | Pro | Asp | Ile | Asp | Asp | Thr | Ala | Met | Gly | Leu | Arg | Ile | Leu | Arg | Leu | | | | | |
| 400 | | | | | 405 | | | | | 410 | | | | | 415 | | | | | |

| | |
|---|------|
| cat gga tac aat gta tcc tca gat gtt tta aaa aca ttt aga gat gag | 1295 |
| His Gly Tyr Asn Val Ser Ser Asp Val Leu Lys Thr Phe Arg Asp Glu | |
| 420 425 430 | |
| aat ggg gag ttc ttt tgc ttc ttg ggt caa aca cag aga gga gtt aca | 1343 |
| Asn Gly Glu Phe Phe Cys Phe Leu Gly Gln Thr Gln Arg Gly Val Thr | |
| 435 440 445 | |
| gac atg tta aac gtc aat cgt tgt tca cat gtt tca ttt ccg gga gaa | 1391 |
| Asp Met Leu Asn Val Asn Arg Cys Ser His Val Ser Phe Pro Gly Glu | |
| 450 455 460 | |
| acg atc atg gaa gaa gca aaa ctc tgt acc gaa agg tat ctg agg aat | 1439 |
| Thr Ile Met Glu Glu Ala Lys Leu Cys Thr Glu Arg Tyr Leu Arg Asn | |
| 465 470 475 | |
| gct ctg gaa aat gtg gat gcc ttt gac aaa tgg gct ttt aaa aag aat | 1487 |
| Ala Leu Glu Asn Val Asp Ala Phe Asp Lys Trp Ala Phe Lys Lys Asn | |
| 480 485 490 495 | |
| att cgg gga gag gta gag tat gca ctc aaa tat ccc tgg cat aag agt | 1535 |
| Ile Arg Gly Glu Val Glu Tyr Ala Leu Lys Tyr Pro Trp His Lys Ser | |
| 500 505 510 | |
| atg cca agg ttg gag gct aga agc tat att gaa aac tat ggg cca gat | 1583 |
| Met Pro Arg Leu Glu Ala Arg Ser Tyr Ile Glu Asn Tyr Gly Pro Asp | |
| 515 520 525 | |
| gat gtg tgg ctt gga aaa act gta tat atg atg cca tac att tcg aat | 1631 |
| Asp Val Trp Leu Gly Lys Thr Val Tyr Met Met Pro Tyr Ile Ser Asn | |
| 530 535 540 | |
| gaa aag tat tta gaa cta gcg aaa ctg gac ttc aat aag gtg cag tct | 1679 |
| Glu Lys Tyr Leu Glu Leu Ala Lys Leu Asp Phe Asn Lys Val Gln Ser | |
| 545 550 555 | |
| ata cac caa aca gag ctt caa gat ctt cga agg tgg tgg aaa tca tcc | 1727 |
| Ile His Gln Thr Glu Leu Gln Asp Leu Arg Arg Trp Trp Lys Ser Ser | |
| 560 565 570 575 | |
| ggt ttc acg gat ctg aat ttc act cgt gag cgt gtg acg gaa ata tat | 1775 |
| Gly Phe Thr Asp Leu Asn Phe Thr Arg Glu Arg Val Thr Glu Ile Tyr | |
| 580 585 590 | |
| ttc tca ccg gca tcc ttt atc ttt gag ccc gag ttt tct aag tgc aga | 1823 |
| Phe Ser Pro Ala Ser Phe Ile Phe Glu Pro Glu Phe Ser Lys Cys Arg | |
| 595 600 605 | |
| gag gtt tat aca aaa act tcc aat ttc act gtt att tta gat gat ctt | 1871 |
| Glu Val Tyr Thr Lys Thr Ser Asn Phe Thr Val Ile Leu Asp Asp Leu | |
| 610 615 620 | |

| | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|
| tat | gac | gcc | cat | gga | tct | tta | gac | gat | ctt | aag | ttg | ttc | aca | gaa | tca | 1919 |
| Tyr | Asp | Ala | His | Gly | Ser | Leu | Asp | Asp | Leu | Lys | Leu | Phe | Thr | Glu | Ser | |
| | 625 | | | | | 630 | | | | | 635 | | | | | |
| gtc | aaa | aga | tgg | gat | cta | tca | cta | gtg | gac | caa | atg | cca | caa | caa | atg | 1967 |
| Val | Lys | Arg | Trp | Asp | Leu | Ser | Leu | Val | Asp | Gln | Met | Pro | Gln | Gln | Met | |
| 640 | | | | | 645 | | | | | 650 | | | | | 655 | |
| aaa | ata | tgt | ttt | gtg | ggg | ttc | tac | aat | act | ttt | aat | gat | ata | gca | aaa | 2015 |
| Lys | Ile | Cys | Phe | Val | Gly | Phe | Tyr | Asn | Thr | Phe | Asn | Asp | Ile | Ala | Lys | |
| | | | | 660 | | | | | 665 | | | | | 670 | | |
| gaa | gga | cgt | gag | agg | caa | ggg | cgc | gat | gtg | cta | ggc | tac | att | caa | aat | 2063 |
| Glu | Gly | Arg | Glu | Arg | Gln | Gly | Arg | Asp | Val | Leu | Gly | Tyr | Ile | Gln | Asn | |
| | | | 675 | | | | | 680 | | | | | 685 | | | |
| gtt | tgg | aaa | gtc | caa | ctt | gaa | gct | tac | acg | aaa | gaa | gca | gaa | tgg | tct | 2111 |
| Val | Trp | Lys | Val | Gln | Leu | Glu | Ala | Tyr | Thr | Lys | Glu | Ala | Glu | Trp | Ser | |
| | | 690 | | | | | 695 | | | | | 700 | | | | |
| gaa | gct | aaa | tat | gtg | cca | tcc | ttc | aat | gaa | tac | ata | gag | aat | gcg | agt | 2159 |
| Glu | Ala | Lys | Tyr | Val | Pro | Ser | Phe | Asn | Glu | Tyr | Ile | Glu | Asn | Ala | Ser | |
| | 705 | | | | | 710 | | | | | 715 | | | | | |
| gtg | tca | ata | gca | ttg | gga | aca | gtc | gtt | ctc | att | agt | gct | ctt | ttc | act | 2207 |
| Val | Ser | Ile | Ala | Leu | Gly | Thr | Val | Val | Leu | Ile | Ser | Ala | Leu | Phe | Thr | |
| 720 | | | | | 725 | | | | | 730 | | | | | 735 | |
| ggg | gag | gtt | ctt | aca | gat | gaa | gta | ctc | tcc | aaa | att | gat | cgc | gaa | tct | 2255 |
| Gly | Glu | Val | Leu | Thr | Asp | Glu | Val | Leu | Ser | Lys | Ile | Asp | Arg | Glu | Ser | |
| | | | | 740 | | | | | 745 | | | | | 750 | | |
| aga | ttt | ctt | caa | ctc | atg | ggc | tta | aca | ggg | cgt | ttg | gtg | aat | gac | acc | 2303 |
| Arg | Phe | Leu | Gln | Leu | Met | Gly | Leu | Thr | Gly | Arg | Leu | Val | Asn | Asp | Thr | |
| | | | 755 | | | | | 760 | | | | | 765 | | | |
| aaa | act | tat | cag | gca | gag | aga | ggg | caa | ggg | gag | gtg | gct | tct | gcc | ata | 2351 |
| Lys | Thr | Tyr | Gln | Ala | Glu | Arg | Gly | Gln | Gly | Glu | Val | Ala | Ser | Ala | Ile | |
| | | 770 | | | | | 775 | | | | | 780 | | | | |
| caa | tgt | tat | atg | aag | gac | cat | cct | aaa | atc | tct | gaa | gaa | gaa | gct | cta | 2399 |
| Gln | Cys | Tyr | Met | Lys | Asp | His | Pro | Lys | Ile | Ser | Glu | Glu | Glu | Ala | Leu | |
| | 785 | | | | | 790 | | | | | 795 | | | | | |
| caa | cat | gtc | tat | agt | gtc | atg | gaa | aat | gcc | ctc | gaa | gag | ttg | aat | agg | 2447 |
| Gln | His | Val | Tyr | Ser | Val | Met | Glu | Asn | Ala | Leu | Glu | Glu | Leu | Asn | Arg | |
| 800 | | | | | 805 | | | | | 810 | | | | | 815 | |
| gag | ttt | gtg | aat | aac | aaa | ata | ccg | gat | att | tac | aaa | aga | ctg | gtt | ttt | 2495 |
| Glu | Phe | Val | Asn | Asn | Lys | Ile | Pro | Asp | Ile | Tyr | Lys | Arg | Leu | Val | Phe | |
| | | | | 820 | | | | | 825 | | | | | 830 | | |
| gaa | act | gca | aga | ata | atg | caa | ctc | ttt | tat | atg | caa | ggg | gat | ggg | ttg | 2543 |

Glu Thr Ala Arg Ile Met Gln Leu Phe Tyr Met Gln Gly Asp Gly Leu
835 840 845

aca cta tca cat gat atg gaa att aaa gag cat gtc aaa aat tgc ctc 2591
Thr Leu Ser His Asp Met Glu Ile Lys Glu His Val Lys Asn Cys Leu
850 855 860

ttc caa cca gtt gcc tag attaaattat tcagtttaaag gccctcatgg 2639
Phe Gln Pro Val Ala *

865

tattgtgtta acattataat aacagatgct caaaagcttt gagcggtatt tgtaaggct 2699
atctttgttt gtttgttgt ttactgccaa ccaaaaagcg ttcctaaacc tttgaagaca 2759
tttccatcca agagatggag tctacatttt atttatgaga ttgaattatt tcaagagaat 2819
atactacata tattttaaag taaaaaaaaa aaaaaaaaaa aa 2861

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<212> PRT
<213> Abies grandis

<400> 56

Met Ala Met Pro Ser Ser Ser Leu Ser Ser Gln Ile Pro Thr Ala Ala
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His His Leu Thr Ala Asn Ala Gln Ser Ile Pro His Phe Ser Thr Thr
20 25 30
Leu Asn Ala Gly Ser Ser Ala Ser Lys Arg Arg Ser Leu Tyr Leu Arg
35 40 45
Trp Gly Lys Gly Ser Asn Lys Ile Ile Ala Cys Val Gly Glu Gly Gly
50 55 60
Ala Thr Ser Val Pro Tyr Gln Ser Ala Glu Lys Asn Asp Ser Leu Ser
65 70 75 80
Ser Ser Thr Leu Val Lys Arg Glu Phe Pro Pro Gly Phe Trp Lys Asp
85 90 95
Asp Leu Ile Asp Ser Leu Thr Ser Ser His Lys Val Ala Ala Ser Asp
100 105 110
Glu Lys Arg Ile Glu Thr Leu Ile Ser Glu Ile Lys Asn Met Phe Arg
115 120 125
Cys Met Gly Tyr Gly Glu Thr Asn Pro Ser Ala Tyr Asp Thr Ala Trp
130 135 140
Val Ala Arg Ile Pro Ala Val Asp Gly Ser Asp Asn Pro His Phe Pro
145 150 155 160
Glu Thr Val Glu Trp Ile Leu Gln Asn Gln Leu Lys Asp Gly Ser Trp
165 170 175
Gly Glu Gly Phe Tyr Phe Leu Ala Tyr Asp Arg Ile Leu Ala Thr Leu
180 185 190
Ala Cys Ile Ile Thr Leu Thr Leu Trp Arg Thr Gly Glu Thr Gln Val
195 200 205
Gln Lys Gly Ile Glu Phe Phe Arg Thr Gln Ala Gly Lys Met Glu Asp
210 215 220
Glu Ala Asp Ser His Arg Pro Ser Gly Phe Glu Ile Val Phe Pro Ala
225 230 235 240
Met Leu Lys Glu Ala Lys Ile Leu Gly Leu Asp Leu Pro Tyr Asp Leu

| | | | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| Pro | Phe | Leu | Lys | 245 | Gln | Ile | Ile | Glu | Lys | 250 | Arg | Glu | Ala | Lys | Leu | Lys | 255 | Arg |
| | | | 260 | | | | | | 265 | | | | | | 270 | | | |
| Ile | Pro | Thr | Asp | Val | Leu | Tyr | Ala | Leu | Pro | Thr | Thr | Leu | Leu | Tyr | Ser | | | |
| | | 275 | | | | | 280 | | | | | | 285 | | | | | |
| Leu | Glu | Gly | Leu | Gln | Glu | Ile | Val | Asp | Trp | Gln | Lys | Ile | Met | Lys | Leu | | | |
| | | 290 | | | | 295 | | | | | 300 | | | | | | | |
| Gln | Ser | Lys | Asp | Gly | Ser | Phe | Leu | Ser | Ser | Pro | Ala | Ser | Thr | Ala | Ala | | | |
| 305 | | | | | 310 | | | | | 315 | | | | | 320 | | | |
| Val | Phe | Met | Arg | Thr | Gly | Asn | Lys | Lys | Cys | Leu | Asp | Phe | Leu | Asn | Phe | | | |
| | | | 325 | | | | | | 330 | | | | | 335 | | | | |
| Val | Leu | Lys | Lys | Phe | Gly | Asn | His | Val | Pro | Cys | His | Tyr | Pro | Leu | Asp | | | |
| | | | 340 | | | | | 345 | | | | | 350 | | | | | |
| Leu | Phe | Glu | Arg | Leu | Trp | Ala | Val | Asp | Thr | Val | Glu | Arg | Leu | Gly | Ile | | | |
| | | 355 | | | | | 360 | | | | | 365 | | | | | | |
| Asp | Arg | His | Phe | Lys | Glu | Glu | Ile | Lys | Glu | Ala | Leu | Asp | Tyr | Val | Tyr | | | |
| | | 370 | | | | 375 | | | | | 380 | | | | | | | |
| Ser | His | Trp | Asp | Glu | Arg | Gly | Ile | Gly | Trp | Ala | Arg | Glu | Asn | Pro | Val | | | |
| 385 | | | | | 390 | | | | | 395 | | | | | 400 | | | |
| Pro | Asp | Ile | Asp | Asp | Thr | Ala | Met | Gly | Leu | Arg | Ile | Leu | Arg | Leu | His | | | |
| | | | 405 | | | | | 410 | | | | | | 415 | | | | |
| Gly | Tyr | Asn | Val | Ser | Ser | Asp | Val | Leu | Lys | Thr | Phe | Arg | Asp | Glu | Asn | | | |
| | | 420 | | | | | | 425 | | | | | 430 | | | | | |
| Gly | Glu | Phe | Cys | Phe | Leu | Gly | Gln | Thr | Gln | Arg | Gly | Val | Thr | Asp | | | | |
| | | 435 | | | | 440 | | | | | 445 | | | | | | | |
| Met | Leu | Asn | Val | Asn | Arg | Cys | Ser | His | Val | Ser | Phe | Pro | Gly | Glu | Thr | | | |
| | | 450 | | | | 455 | | | | | 460 | | | | | | | |
| Ile | Met | Glu | Glu | Ala | Lys | Leu | Cys | Thr | Glu | Arg | Tyr | Leu | Arg | Asn | Ala | | | |
| 465 | | | | | 470 | | | | | 475 | | | | | 480 | | | |
| Leu | Glu | Asn | Val | Asp | Ala | Phe | Asp | Lys | Trp | Ala | Phe | Lys | Lys | Asn | Ile | | | |
| | | | 485 | | | | | 490 | | | | | | 495 | | | | |
| Arg | Gly | Glu | Val | Glu | Tyr | Ala | Leu | Lys | Tyr | Pro | Trp | His | Lys | Ser | Met | | | |
| | | | 500 | | | | | 505 | | | | | 510 | | | | | |
| Pro | Arg | Leu | Glu | Ala | Arg | Ser | Tyr | Ile | Glu | Asn | Tyr | Gly | Pro | Asp | Asp | | | |
| | | 515 | | | | | 520 | | | | | 525 | | | | | | |
| Val | Trp | Leu | Gly | Lys | Thr | Val | Tyr | Met | Met | Pro | Tyr | Ile | Ser | Asn | Glu | | | |
| | | 530 | | | | 535 | | | | | 540 | | | | | | | |
| Lys | Tyr | Leu | Glu | Leu | Ala | Lys | Leu | Asp | Phe | Asn | Lys | Val | Gln | Ser | Ile | | | |
| 545 | | | | | 550 | | | | | 555 | | | | | 560 | | | |
| His | Gln | Thr | Glu | Leu | Gln | Asp | Leu | Arg | Arg | Trp | Trp | Lys | Ser | Ser | Gly | | | |
| | | | 565 | | | | | | 570 | | | | | 575 | | | | |
| Phe | Thr | Asp | Leu | Asn | Phe | Thr | Arg | Glu | Arg | Val | Thr | Glu | Ile | Tyr | Phe | | | |
| | | | 580 | | | | | 585 | | | | 590 | | | | | | |
| Ser | Pro | Ala | Ser | Phe | Ile | Phe | Glu | Pro | Glu | Phe | Ser | Lys | Cys | Arg | Glu | | | |
| | | 595 | | | | | 600 | | | | | 605 | | | | | | |
| Val | Tyr | Thr | Lys | Thr | Ser | Asn | Phe | Thr | Val | Ile | Leu | Asp | Asp | Leu | Tyr | | | |
| | | 610 | | | | 615 | | | | | 620 | | | | | | | |
| Asp | Ala | His | Gly | Ser | Leu | Asp | Asp | Leu | Lys | Leu | Phe | Thr | Glu | Ser | Val | | | |
| 625 | | | | | 630 | | | | | 635 | | | | | 640 | | | |
| Lys | Arg | Trp | Asp | Leu | Ser | Leu | Val | Asp | Gln | Met | Pro | Gln | Gln | Met | Lys | | | |
| | | | 645 | | | | | | 650 | | | | | 655 | | | | |
| Ile | Cys | Phe | Val | Gly | Phe | Tyr | Asn | Thr | Phe | Asn | Asp | Ile | Ala | Lys | Glu | | | |
| | | | 660 | | | | | 665 | | | | | 670 | | | | | |

Gly Arg Glu Arg Gln Gly Arg Asp Val Leu Gly Tyr Ile Gln Asn Val
 675 680 685
 Trp Lys Val Gln Leu Glu Ala Tyr Thr Lys Glu Ala Glu Trp Ser Glu
 690 695 700
 Ala Lys Tyr Val Pro Ser Phe Asn Glu Tyr Ile Glu Asn Ala Ser Val
 705 710 715 720
 Ser Ile Ala Leu Gly Thr Val Val Leu Ile Ser Ala Leu Phe Thr Gly
 725 730 735
 Glu Val Leu Thr Asp Glu Val Leu Ser Lys Ile Asp Arg Glu Ser Arg
 740 745 750
 Phe Leu Gln Leu Met Gly Leu Thr Gly Arg Leu Val Asn Asp Thr Lys
 755 760 765
 Thr Tyr Gln Ala Glu Arg Gly Gln Gly Glu Val Ala Ser Ala Ile Gln
 770 775 780
 Cys Tyr Met Lys Asp His Pro Lys Ile Ser Glu Glu Glu Ala Leu Gln
 785 790 795 800
 His Val Tyr Ser Val Met Glu Asn Ala Leu Glu Glu Leu Asn Arg Glu
 805 810 815
 Phe Val Asn Asn Lys Ile Pro Asp Ile Tyr Lys Arg Leu Val Phe Glu
 820 825 830
 Thr Ala Arg Ile Met Gln Leu Phe Tyr Met Gln Gly Asp Gly Leu Thr
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 Leu Ser His Asp Met Glu Ile Lys Glu His Val Lys Asn Cys Leu Phe
 850 855 860
 Gln Pro Val Ala
 865

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 aggcaggaat cc atg gct ctc ctt tct atc gta tct ttg cag gtt ccc aaa 111
 Met Ala Leu Leu Ser Ile Val Ser Leu Gln Val Pro Lys
 1 5 10

 tcc tgc ggg ctg aaa tcg ttg atc agt tcc agc aat gtg cag aag gct 159
 Ser Cys Gly Leu Lys Ser Leu Ile Ser Ser Ser Asn Val Gln Lys Ala
 15 20 25

 ctc tgt atc tct aca gca gtc cca aca ctc aga atg cgt agg cga cag 207
 Leu Cys Ile Ser Thr Ala Val Pro Thr Leu Arg Met Arg Arg Arg Gln
 30 35 40 45

 aaa gct ctg gtc atc aac atg aaa ttg acc act gta tcc cat cgt gat 255
 Lys Ala Leu Val Ile Asn Met Lys Leu Thr Thr Val Ser His Arg Asp

| 50 | | | | | | | | | | 55 | | | | | 60 | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|--|--|--|--|
| gat | aat | ggt | ggt | ggt | gta | ctg | caa | aga | cgc | ata | gcc | gat | cat | cat | ccc | 303 | | | | |
| Asp | Asn | Gly | Gly | Gly | Val | Leu | Gln | Arg | Arg | Ile | Ala | Asp | His | His | Pro | | | | | |
| | | | 65 | | | | | 70 | | | | | 75 | | | | | | | |
| aac | ctg | tgg | gaa | gat | gat | ttc | ata | caa | tca | ttg | tcc | tca | cct | tat | ggg | 351 | | | | |
| Asn | Leu | Trp | Glu | Asp | Asp | Phe | Ile | Gln | Ser | Leu | Ser | Ser | Pro | Tyr | Gly | | | | | |
| | | 80 | | | | | 85 | | | | | 90 | | | | | | | | |
| gga | tct | tcg | tac | agt | gaa | cgt | gct | gag | aca | gtc | gtt | gag | gaa | gta | aaa | 399 | | | | |
| Gly | Ser | Ser | Tyr | Ser | Glu | Arg | Ala | Glu | Thr | Val | Val | Glu | Glu | Val | Lys | | | | | |
| | 95 | | | | | 100 | | | | | 105 | | | | | | | | | |
| gag | atg | ttc | aat | tca | ata | cca | aat | aat | aga | gaa | tta | ttt | ggt | tcc | caa | 447 | | | | |
| Glu | Met | Phe | Asn | Ser | Ile | Pro | Asn | Asn | Arg | Glu | Leu | Phe | Gly | Ser | Gln | | | | | |
| 110 | | | | | 115 | | | | | 120 | | | | | 125 | | | | | |
| aat | gat | ctc | ctt | aca | cgc | ctt | tgg | atg | gtg | gat | agc | att | gaa | cgt | ctg | 495 | | | | |
| Asn | Asp | Leu | Leu | Thr | Arg | Leu | Trp | Met | Val | Asp | Ser | Ile | Glu | Arg | Leu | | | | | |
| | | | | 130 | | | | | 135 | | | | | 140 | | | | | | |
| ggg | ata | gat | aga | cat | ttc | caa | aat | gag | ata | aga | gta | gcc | ctc | gat | tat | 543 | | | | |
| Gly | Ile | Asp | Arg | His | Phe | Gln | Asn | Glu | Ile | Arg | Val | Ala | Leu | Asp | Tyr | | | | | |
| | | | 145 | | | | | 150 | | | | | 155 | | | | | | | |
| gtt | tac | agt | tat | tgg | aag | gaa | aag | gaa | ggc | att | ggg | tgt | ggc | aga | gat | 591 | | | | |
| Val | Tyr | Ser | Tyr | Trp | Lys | Glu | Lys | Glu | Gly | Ile | Gly | Cys | Gly | Arg | Asp | | | | | |
| | | 160 | | | | | 165 | | | | | 170 | | | | | | | | |
| tct | act | ttt | cct | gat | ctc | aac | tcg | act | gcc | ttg | gcg | ctt | cga | act | ctt | 639 | | | | |
| Ser | Thr | Phe | Pro | Asp | Leu | Asn | Ser | Thr | Ala | Leu | Ala | Leu | Arg | Thr | Leu | | | | | |
| | 175 | | | | | 180 | | | | | 185 | | | | | | | | | |
| cga | ctg | cac | gga | tac | aat | gtg | tct | tca | gat | gtg | ctg | gaa | tac | ttc | aaa | 687 | | | | |
| Arg | Leu | His | Gly | Tyr | Asn | Val | Ser | Ser | Asp | Val | Leu | Glu | Tyr | Phe | Lys | | | | | |
| 190 | | | | | 195 | | | | | 200 | | | | | 205 | | | | | |
| gat | gaa | aag | ggg | cat | ttt | gcc | tgc | cct | gca | atc | cta | acc | gag | gga | cag | 735 | | | | |
| Asp | Glu | Lys | Gly | His | Phe | Ala | Cys | Pro | Ala | Ile | Leu | Thr | Glu | Gly | Gln | | | | | |
| | | | | 210 | | | | | 215 | | | | | 220 | | | | | | |
| atc | act | aga | agt | gtt | cta | aat | tta | tat | cgg | gct | tcc | ctg | gtc | gcc | ttt | 783 | | | | |
| Ile | Thr | Arg | Ser | Val | Leu | Asn | Leu | Tyr | Arg | Ala | Ser | Leu | Val | Ala | Phe | | | | | |
| | | | 225 | | | | | 230 | | | | | 235 | | | | | | | |
| ccc | ggg | gag | aaa | gtt | atg | gaa | gag | gct | gaa | atc | ttc | tcg | gca | tct | tat | 831 | | | | |
| Pro | Gly | Glu | Lys | Val | Met | Glu | Glu | Ala | Glu | Ile | Phe | Ser | Ala | Ser | Tyr | | | | | |
| | | 240 | | | | | 245 | | | | | 250 | | | | | | | | |
| ttg | aaa | aaa | gtc | tta | caa | aag | att | ccg | gtc | tcc | aat | ctt | tca | gga | gag | 879 | | | | |
| Leu | Lys | Lys | Val | Leu | Gln | Lys | Ile | Pro | Val | Ser | Asn | Leu | Ser | Gly | Glu | | | | | |
| | 255 | | | | | 260 | | | | | 265 | | | | | | | | | |

| | |
|---|------|
| ata gaa tat gtt ttg gaa tat ggt tgg cac acg aat ttg ccg aga ttg Ile Glu Tyr Val Leu Glu Tyr Gly Trp His Thr Asn Leu Pro Arg Leu 270 275 280 285 | 927 |
| gaa gca aga aat tat atc gag gtc tac gag cag agc ggc tat gaa agc Glu Ala Arg Asn Tyr Ile Glu Val Tyr Glu Gln Ser Gly Tyr Glu Ser 290 295 300 | 975 |
| tta aac gag atg cca tat atg aac atg aag aag ctt tta caa ctt gca Leu Asn Glu Met Pro Tyr Met Asn Met Lys Lys Leu Leu Gln Leu Ala 305 310 315 | 1023 |
| aaa ttg gag ttc aat atc ttt cac tct ttg caa cta aga gag tta caa Lys Leu Glu Phe Asn Ile Phe His Ser Leu Gln Leu Arg Glu Leu Gln 320 325 330 | 1071 |
| tct atc tcc aga tgg tgg aaa gaa tca ggt tcg tct caa ctg act ttt Ser Ile Ser Arg Trp Trp Lys Glu Ser Gly Ser Ser Gln Leu Thr Phe 335 340 345 | 1119 |
| aca cgg cat cgt cac gtg gaa tac tac act atg gca tct tgc att tct Thr Arg His Arg His Val Glu Tyr Tyr Thr Met Ala Ser Cys Ile Ser 350 355 360 365 | 1167 |
| atg ttg cca aaa cat tca gct ttc aga atg gag ttt gtc aaa gtg tgt Met Leu Pro Lys His Ser Ala Phe Arg Met Glu Phe Val Lys Val Cys 370 375 380 | 1215 |
| cat ctt gta aca gtt ctc gat gat ata tat gac act ttt gga aca atg His Leu Val Thr Val Leu Asp Asp Ile Tyr Asp Thr Phe Gly Thr Met 385 390 395 | 1263 |
| aac gaa ctc caa ctt ttt acg gat gca att aag aga tgg gat ttg tca Asn Glu Leu Gln Leu Phe Thr Asp Ala Ile Lys Arg Trp Asp Leu Ser 400 405 410 | 1311 |
| acg aca agg tgg ctt cca gaa tat atg aaa gga gtg tac atg gac ttg Thr Thr Arg Trp Leu Pro Glu Tyr Met Lys Gly Val Tyr Met Asp Leu 415 420 425 | 1359 |
| tat caa tgc att aat gaa atg gtg gaa gag gct gag aag act caa ggc Tyr Gln Cys Ile Asn Glu Met Val Glu Glu Ala Glu Lys Thr Gln Gly 430 435 440 445 | 1407 |
| cga gat atg ctc aac tat att caa aat gct tgg gaa gcc cta ttt gat Arg Asp Met Leu Asn Tyr Ile Gln Asn Ala Trp Glu Ala Leu Phe Asp 450 455 460 | 1455 |
| acc ttt atg caa gaa gca aag tgg atc tcc agc agt tat ctc cca acg Thr Phe Met Gln Glu Ala Lys Trp Ile Ser Ser Ser Tyr Leu Pro Thr 465 470 475 | 1503 |

| | |
|---|------|
| ttt gag gag tac ttg aag aat gca aaa gtt agt tct ggt tct cgc ata | 1551 |
| Phe Glu Glu Tyr Leu Lys Asn Ala Lys Val Ser Ser Gly Ser Arg Ile | |
| 480 485 490 | |
| gcc aca tta caa ccc att ctc act ttg gat gta cca ctt cct gat tac | 1599 |
| Ala Thr Leu Gln Pro Ile Leu Thr Leu Asp Val Pro Leu Pro Asp Tyr | |
| 495 500 505 | |
| ata ctg caa gaa att gat tat cca tcc aga ttc aat gag tta gct tcg | 1647 |
| Ile Leu Gln Glu Ile Asp Tyr Pro Ser Arg Phe Asn Glu Leu Ala Ser | |
| 510 515 520 525 | |
| tcc atc ctt cga cta cga ggt gac acg cgc tgc tac aag gcg gat agg | 1695 |
| Ser Ile Leu Arg Leu Arg Gly Asp Thr Arg Cys Tyr Lys Ala Asp Arg | |
| 530 535 540 | |
| gcc cgt gga gaa gaa gct tca gct ata tcg tgt tat atg aaa gac cat | 1743 |
| Ala Arg Gly Glu Glu Ala Ser Ala Ile Ser Cys Tyr Met Lys Asp His | |
| 545 550 555 | |
| cct gga tca ata gag gaa gat gct ctc aat cat atc aac gcc atg atc | 1791 |
| Pro Gly Ser Ile Glu Glu Asp Ala Leu Asn His Ile Asn Ala Met Ile | |
| 560 565 570 | |
| agt gat gca atc aga gaa tta aat tgg gag ctt ctc aga ccg gat agc | 1839 |
| Ser Asp Ala Ile Arg Glu Leu Asn Trp Glu Leu Leu Arg Pro Asp Ser | |
| 575 580 585 | |
| aaa agt ccc atc tct tcc aag aaa cat gct ttt gac atc acc aga gct | 1887 |
| Lys Ser Pro Ile Ser Ser Lys Lys His Ala Phe Asp Ile Thr Arg Ala | |
| 590 595 600 605 | |
| ttc cat cat gtc tac aaa tat cga gat ggt tac act gtt tcc aac aac | 1935 |
| Phe His His Val Tyr Lys Tyr Arg Asp Gly Tyr Thr Val Ser Asn Asn | |
| 610 615 620 | |
| gaa aca aag aat ttg gtg atg aaa acc gtt ctt gaa cct ctc gct ttg | 1983 |
| Glu Thr Lys Asn Leu Val Met Lys Thr Val Leu Glu Pro Leu Ala Leu | |
| 625 630 635 | |
| taa aaacatatag aatgcattaa aatgtgggaa gtctataatc tagactattc | 2036 |
| * | |
| tctatctttc ataatgtaga tctggatgtg tattgaactc taaaaaaaaa aaa | 2089 |
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| <211> 637 | |
| <212> PRT | |
| <213> Abies grandis | |
| <400> 58 | |
| Met Ala Leu Leu Ser Ile Val Ser Leu Gln Val Pro Lys Ser Cys Gly | |

| | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| 1 | Leu | Lys | Ser | Leu | Ile | Ser | Ser | Ser | Asn | Val | Gln | Lys | Ala | Leu | Cys | Ile |
| | | | | 20 | | | | | 25 | | | | | 30 | | |
| | Ser | Thr | Ala | Val | Pro | Thr | Leu | Arg | Met | Arg | Arg | Arg | Gln | Lys | Ala | Leu |
| | | | 35 | | | | | 40 | | | | | 45 | | | |
| | Val | Ile | Asn | Met | Lys | Leu | Thr | Thr | Val | Ser | His | Arg | Asp | Asp | Asn | Gly |
| | | 50 | | | | | 55 | | | | | 60 | | | | |
| | Gly | Gly | Val | Leu | Gln | Arg | Arg | Ile | Ala | Asp | His | His | Pro | Asn | Leu | Trp |
| 65 | | | | | 70 | | | | | | 75 | | | | 80 | |
| | Glu | Asp | Asp | Phe | Ile | Gln | Ser | Leu | Ser | Ser | Pro | Tyr | Gly | Gly | Ser | Ser |
| | | | | 85 | | | | | | 90 | | | | | 95 | |
| | Tyr | Ser | Glu | Arg | Ala | Glu | Thr | Val | Val | Glu | Glu | Val | Lys | Glu | Met | Phe |
| | | | | 100 | | | | | 105 | | | | | 110 | | |
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| | Leu | Thr | Arg | Leu | Trp | Met | Val | Asp | Ser | Ile | Glu | Arg | Leu | Gly | Ile | Asp |
| | | 130 | | | | | 135 | | | | | 140 | | | | |
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| | Tyr | Trp | Lys | Glu | Lys | Glu | Gly | Ile | Gly | Cys | Gly | Arg | Asp | Ser | Thr | Phe |
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| | Pro | Asp | Leu | Asn | Ser | Thr | Ala | Leu | Ala | Leu | Arg | Thr | Leu | Arg | Leu | His |
| | | | | 180 | | | | | 185 | | | | | 190 | | |
| | Gly | Tyr | Asn | Val | Ser | Ser | Asp | Val | Leu | Glu | Tyr | Phe | Lys | Asp | Glu | Lys |
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| | Phe | Asn | Ile | Phe | His | Ser | Leu | Gln | Leu | Arg | Glu | Leu | Gln | Ser | Ile | Ser |
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| | | | | 405 | | | | | | 410 | | | | | 415 | |
| | Trp | Leu | Pro | Glu | Tyr | Met | Lys | Gly | Val | Tyr | Met | Asp | Leu | Tyr | Gln | Cys |
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| | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
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| 465 | | | | | 470 | | | | | 475 | | | | | 480 |
| Tyr | Leu | Lys | Asn | Ala | Lys | Val | Ser | Ser | Gly | Ser | Arg | Ile | Ala | Thr | Leu |
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| Gln | Pro | Ile | Leu | Thr | Leu | Asp | Val | Pro | Leu | Pro | Asp | Tyr | Ile | Leu | Gln |
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| Arg | Leu | Arg | Gly | Asp | Thr | Arg | Cys | Tyr | Lys | Ala | Asp | Arg | Ala | Arg | Gly |
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| Glu | Glu | Ala | Ser | Ala | Ile | Ser | Cys | Tyr | Met | Lys | Asp | His | Pro | Gly | Ser |
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| Asn | Leu | Val | Met | Lys | Thr | Val | Leu | Glu | Pro | Leu | Ala | Leu | | | |
| 625 | | | | | 630 | | | | | 635 | | | | | |

INTERNATIONAL SEARCH REPORT

International Application No
PCT/US 99/21419

A. CLASSIFICATION OF SUBJECT MATTER

IPC 7 C12N9/10 C07K14/415 C12N15/54 C12N15/29 C12N9/88

According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)

IPC 7 C12N C07K

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practical, search terms used)

C. DOCUMENTS CONSIDERED TO BE RELEVANT

| Category | Citation of document, with indication, where appropriate, of the relevant passages | Relevant to claim No. |
|----------|--|-----------------------|
| X | STARKS, C.M. ET AL: "Structural basis for cyclic terpene biosynthesis by tobacco 5-epi-aristolochene synthase" SCIENCE, vol. 277, 19 September 1997 (1997-09-19), pages 1815-1820, XP000867114 LANCASTER US the whole document | 1-94 |
| X | WO 97 38703 A (UNIVERSITY OF KENTUCKY) 23 October 1997 (1997-10-23) the whole document | 95-101, 144, 153 |

☒ Further documents are listed in the continuation of box C.

☒ Patent family members are listed in annex.

* Special categories of cited documents:

- *A* document defining the general state of the art which is not considered to be of particular relevance
- *E* earlier document but published on or after the international filing date
- *L* document which may throw doubts on priority claim(s) or which is cited to establish the publication date of another citation or other special reason (as specified)
- *O* document referring to an oral disclosure, use, exhibition or other means
- *P* document published prior to the international filing date but later than the priority date claimed

T later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention

- *X* document of particular relevance; the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone
- *Y* document of particular relevance; the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art.

* & * document member of the same patent family

Date of the actual completion of the international search

9 February 2000

Date of mailing of the international search report

23. MAI 2000

Name and mailing address of the ISA

European Patent Office, P.B. 5818 Patentlaan 2
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Authorized officer

De Kok, A

INTERNATIONAL SEARCH REPORT

International Application No.
PCT/US 99/21419

| C.(Continuation) DOCUMENTS CONSIDERED TO BE RELEVANT | | |
|--|--|-----------------------|
| Category * | Citation of document, with indication, where appropriate, of the relevant passages | Relevant to claim No. |
| A | <p>LESBURG C.A. ET AL.: "Crystal structure of pentalene synthase: mechanistic insights on terpenoid cyclization reactions in biology" SCIENCE., vol. 277, no. 5333, 19 September 1997 (1997-09-19), pages 1820-1824, XP000867083 LANCASTER US the whole document</p> | 1 |
| A | <p>MAU C.J.D. ET AL.: "Cloning of casbene synthase cDNA: evidence for conserved structural features among terpenoid cyclases in plants" PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF USA., vol. 91, August 1994 (1994-08), pages 8497-8501, XP002130098 WASHINGTON US ISSN: 0027-8424 the whole document</p> | 1 |
| A | <p>PETER FACCHINI ET AL.: "Gene family for an elicitor-induced sesquiterpene cyclase in tobacco" PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF USA,US,NATIONAL ACADEMY OF SCIENCE. WASHINGTON, vol. 89, no. 89, page 11088-11092-11092 XP002102270 ISSN: 0027-8424 the whole document</p> | 1 |
| A | <p>WO 96 36697 A (UNIVERSITY OF KENTUCKY) 21 November 1996 (1996-11-21) page 19, line 1 -page 44, line 14</p> | 1 |
| P,X | <p>LESBURG C.A. ET AL.: "Managing and manipulating carbocations in biology: Terpenoid cyclase structure and mechanism" CURRENT OPINION IN STRUCTURAL BIOLOGY., vol. 8, no. 6, December 1998 (1998-12), pages 695-703, XP000874866 LONDON GB ISSN: 0959-440X the whole document</p> | 1 |

INTERNATIONAL SEARCH REPORT

International application No.
PCT/US 99/21419

Box I Observations where certain claims were found unsearchable (Continuation of item 1 of first sheet)

This International Search Report has not been established in respect of certain claims under Article 17(2)(a) for the following reasons:

1. ☐ Claims Nos.:
because they relate to subject matter not required to be searched by this Authority, namely:
2. ☒ Claims Nos.:
because they relate to parts of the International Application that do not comply with the prescribed requirements to such an extent that no meaningful International Search can be carried out, specifically:
see FURTHER INFORMATION sheet PCT/ISA/210
3. ☐ Claims Nos.:
because they are dependent claims and are not drafted in accordance with the second and third sentences of Rule 6.4(a).

Box II Observations where unity of invention is lacking (Continuation of item 2 of first sheet)

This International Searching Authority found multiple inventions in this international application, as follows:

1. ☐ As all required additional search fees were timely paid by the applicant, this International Search Report covers all searchable claims.
2. ☐ As all searchable claims could be searched without effort justifying an additional fee, this Authority did not invite payment of any additional fee.
3. ☐ As only some of the required additional search fees were timely paid by the applicant, this International Search Report covers only those claims for which fees were paid, specifically claims Nos.:
4. ☒ No required additional search fees were timely paid by the applicant. Consequently, this International Search Report is restricted to the invention first mentioned in the claims; it is covered by claims Nos.:
1-101, 119-128, 129-132 PARTLY, 133-151, 153-162

Remark on Protest

- ☐ The additional search fees were accompanied by the applicant's protest.
- ☐ No protest accompanied the payment of additional search fees.

FURTHER INFORMATION CONTINUED FROM PCT/ISA/ 210

Continuation of Box I.2

Present claims 1-101, 119-151, 153-162 relate to an extremely large number of possible compounds i.e. terpene synthases. In fact, the claims contain so many options, variables, possible permutations and provisos that a lack of clarity (and/or conciseness) within the meaning of Article 6 PCT arises to such an extent as to render a meaningful search of the claims impossible. Consequently, the search has been carried out for those parts of the application which do appear to be clear (and/or concise), namely those terpene synthases recited in examples 1-10.

The applicant's attention is drawn to the fact that claims, or parts of claims, relating to inventions in respect of which no international search report has been established need not be the subject of an international preliminary examination (Rule 66.1(e) PCT). The applicant is advised that the EPO policy when acting as an International Preliminary Examining Authority is normally not to carry out a preliminary examination on matter which has not been searched. This is the case irrespective of whether or not the claims are amended following receipt of the search report or during any Chapter II procedure.

FURTHER INFORMATION CONTINUED FROM PCT/ISA/ 210

1. Claims: 1-101, 119-128, 129-132 partly, 133-151, 153-162

Isolated terpene synthases having a region with 20% or greater sequence identity to residues 265 to 535 of SEQ.ID.NO:2 (tobacco 5-epi-aristolochene synthase) and having an ordered arrangement of R-groups at active-center alpha-carbons other than those characterized in Tables 7-9; fusion proteins comprising said terpene synthases; methods for making said terpene synthases; nucleic acids encoding said terpene synthases; host cells containing said nucleic acids; transgenic plants containing said nucleic acids and transgenic animal cell cultures containing said nucleic acids.

2. Claims: 102, 129 partly, 130 partly, 152 partly

An isolated synthase having 40% or greater sequence identity to residues 343 to 612 of SEQ.ID.NO: 20 (pinene synthase) having an arrangement of amino acid residues at active site positions other than a range of specified ordered arrangements (see page 290 description); method for synthesizing said synthase and an isolated nucleic acid encoding said synthase.

3. Claims: 103, 152 partly

An isolated synthase having 40% or greater sequence identity to residues 316 to 586 of SEQ.ID.NO: 22 (spearmint limonene synthase) having an arrangement of amino acid residues at active site positions other than a range of specified ordered arrangements (see page 292 description); method for synthesizing said synthase and an isolated nucleic acid encoding said synthase.

4. Claims: 104, 152 partly

An isolated synthase having 40% or greater sequence identity to residues 352 to 622 of SEQ.ID.NO: 58 (grand fir limonene synthase) having an arrangement of amino acid residues at active site positions other than a range of specified ordered arrangements (see page 294 description); method for synthesizing said synthase and an isolated nucleic acid encoding said synthase.

5. Claims: 105, 152 partly

An isolated synthase having 40% or greater sequence identity to residues 272 to 540 of SEQ.ID.NO: 33 (cotton delta catadinene synthase) having an arrangement of amino acid residues at active site positions other than a range of specified ordered arrangements (see page 296 description); method for synthesizing said synthase and an isolated

FURTHER INFORMATION CONTINUED FROM PCT/ISA/ 210

nucleic acid encoding said synthase.

6. Claims: 106, 152 partly

An isolated synthase having 40% or greater sequence identity to residues 319 to 571 of SEQ.ID.NO: 42 (castor bean casbene synthase) having an arrangement of amino acid residues at active site positions other than a range of specified ordered arrangements (see page 298 description); method for synthesizing said synthase and an isolated nucleic acid encoding said synthase.

7. Claims: 107, 131 partly, 132 partly, 152 partly

An isolated synthase having 40% or greater sequence identity to residues 579 to 847 of SEQ.ID.NO: 44 (yew taxadiene synthase) having an arrangement of amino acid residues at active site positions other than a range of specified ordered arrangements (see page 300 description); method for synthesizing said synthase and an isolated nucleic acid encoding said synthase.

8. Claims: 108, 152 partly

An isolated synthase having 40% or greater sequence identity to residues 495 to 767 of SEQ.ID.NO: 46 (grand fir E-alpha bisabolene synthase) having an arrangement of amino acid residues at active site positions other than a range of specified ordered arrangements (see page 302 description); method for synthesizing said synthase and an isolated nucleic acid encoding said synthase.

9. Claims: 109, 152 partly

An isolated synthase having 40% or greater sequence identity to residues 295 to 564 of SEQ.ID.NO: 48 (grand fir delta selinene synthase) having an arrangement of amino acid residues at active site positions other than a range of specified ordered arrangements (see page 304 description); method for synthesizing said synthase and an isolated nucleic acid encoding said synthase.

10. Claims: 110, 152 partly

An isolated synthase having 40% or greater sequence identity to residues 307 to 578 of SEQ.ID.NO: 50 (grand fir gamma humulene synthase) having an arrangement of amino acid residues at active site positions other than a range of specified ordered arrangements (see page 306 description); method for synthesizing said synthase and an isolated

FURTHER INFORMATION CONTINUED FROM PCT/ISA/ 210

nucleic acid encoding said synthase.

11. Claims: 111, 152 partly

An isolated synthase having 40% or greater sequence identity to residues 264 to 533 of SEQ.ID.NO: 52 (tomato germacrene synthase) having an arrangement of amino acid residues at active site positions other than a range of specified ordered arrangements (see page 308 description); method for synthesizing said synthase and an isolated nucleic acid encoding said synthase.

12. Claims: 112, 152 partly

An isolated synthase having 40% or greater sequence identity to residues 585 to 853 of SEQ.ID.NO: 56 (grand fir abiatadiene synthase) having an arrangement of amino acid residues at active site positions other than a range of specified ordered arrangements (see page 310 description); method for synthesizing said synthase and an isolated nucleic acid encoding said synthase.

13. Claims: 113, 152 partly

An isolated synthase having 40% or greater sequence identity to residues 307 to 574 of SEQ.ID.NO: 54 (sage +sabinene synthase) having an arrangement of amino acid residues at active site positions other than a range of specified ordered arrangements (see page 312 description); method for synthesizing said synthase and an isolated nucleic acid encoding said synthase.

14. Claims: 114, 152 partly

An isolated synthase having 40% or greater sequence identity to residues 309 to 577 of SEQ.ID.NO: 24 (sage 1,8-cineole synthase) having an arrangement of amino acid residues at active site positions other than a range of specified ordered arrangements (see page 314 description); method for synthesizing said synthase and an isolated nucleic acid encoding said synthase.

15. Claims: 115, 152 partly

An isolated synthase having 40% or greater sequence identity to residues 315 to 584 of SEQ.ID.NO: 26 (sage bornyl diphosphate synthase) having an arrangement of amino acid residues at active site positions other than a range of specified ordered arrangements (see page 316 description); method for synthesizing said synthase and an isolated

FURTHER INFORMATION CONTINUED FROM PCT/ISA/ 210

nucleic acid encoding said synthase.

16. Claims: 116, 152 partly

An isolated synthase having 40% or greater sequence identity to residues 265 to 536 of SEQ.ID.NO: 28 (mint E-b-farnesene synthase) having an arrangement of amino acid residues at active site positions other than a range of specified ordered arrangements (see page 318 description); method for synthesizing said synthase and an isolated nucleic acid encoding said synthase.

17. Claims: 117, 152 partly

An isolated synthase having 40% or greater sequence identity to residues 342 to 612 of SEQ.ID.NO: 30 (grand fir myrcene synthase) having an arrangement of amino acid residues at active site positions other than a range of specified ordered arrangements (see page 320 description); method for synthesizing said synthase and an isolated nucleic acid encoding said synthase.

18. Claims: 118, 152 partly

An isolated synthase having 40% or greater sequence identity to residues 307 to 541 of SEQ.ID.NO: 32 (potato vetaspiradiene synthase) having an arrangement of amino acid residues at active site positions other than a range of specified ordered arrangements (see page 322 description); method for synthesizing said synthase and an isolated nucleic acid encoding said synthase.

INTERNATIONAL SEARCH REPORT

information on patent family members

International Application No

PCT/US 99/21419

| Patent document cited in search report | | Publication date | Patent family member(s) | Publication date |
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| ----- | | | | |